SPSAS NanoAgri&Enviro

São Paulo School of Advanced Science on Nanotechnology, Agriculture & Environment

3rd to 15th of July 2023
Campinas, SP – Brazil

ABSTRACT BOOK

Funded by FAPESP São Paulo Research Foundation

Organized by CNPEM Centro Nacional de Pesquisa em Energia e Materiais; Ministério da Ciência, Tecnologia e Inovação; Governo Federal Brasil União e Reconstrução

Co-organized by USP; unesp; ufscar; Embrapa; UNISO

Sponsored by SisNANO MCTI Brazilian System of Laboratories in Nanotechnologies; ThermoFisher Scientific; IBM; Malvern Panalytical

SUMMARY

PREFACE

This book of abstracts is a contribution of participants to the **São Paulo School of Advanced Science on Nanotechnology, Agriculture & Environment (SPSAS NanoAgri&Enviro)**, which was held on 3-15 July 2023 at the Brazilian Center for Research in Energy and Materials in Campinas, São Paulo, Brazil.

The SPSAS NanoAgri&Enviro gathered 87 selected participants from 24 countries and 14 Brazilian states. We believe that this diversity linked to the excellent academic background of all participants and speakers greatly enriched the quality of school.

The SPSAS NanoAgri&Enviro was an opportunity for participants to discuss the most recent scientific findings, fundamentals and perspectives regarding nanotechnology and cross-interdisciplinary fields such as agriculture and foods, the environment, surface and colloidal chemistry, materials characterization, computational modeling and nanoinformatics. Developing safe and sustainable nano advanced materials is a challenge; we hope of this school will encourage the participants keep this in mind during your actions in research, institutes, job positions and future society interactions.

Special thanks must be directed to all members of committees, session moderators and colleagues for their help and contribution to our school's success. We extend gratitude to the following institutions for supporting this school: CNPEM, UNESP, USP, EMBRAPA, UFSCar and UNISO.

Very special thanks to the Sao Paulo Research Foundation (FAPESP) for funding (Proc. No. 22/05207-1) and to the official sponsors of this advanced school: Themo Fisher, IBM, Malvern Panalytical and SisNANO/MCTI.

Thank you very much for all participants and speakers that makes SPSAS NanoAgri&Enviro a great experience and an excellent learning environment

Dr. Diego Stéfani Teodoro Martinez

SPSAS NanoAgri&Enviro – Chair

Campinas, SP

Enabling simultaneous valorization of tannery effluent and waste plastic for sustainably preparing MOFs useful for water adsorption

Achraf Delhali[1], Ayalew H. Assen[1,2,*] , Aminat Mohammed[2], Karim Adil[1,3], Youssef Belmabkhout[1,*]

[1] *Applied Chemistry and Engineering Research Centre of Excellence (ACER CoE), Mohammed VI Polytechnic University (UM6P), Lot 660 - Hay Moulay Rachid, 43150 Ben Guerir, Morocco*

[2] *Department of Chemistry, College of Natural Science, Wollo University, Dessie, Ethiopia*

[3] *Le Mans Université, Institut des Molécules et des Matériaux du Mans. Avenue Olivier Messiaen, 72085 Le Mans cedex, France*

** Corresponding authors: Ayalew H. Assen; Y. Belmabkhout*

E-mail address: ayalew.assen@um6p.ma; youssef.belmabkhout@um6p.ma

Metal-organic frameworks (MOFs) are highly porous materials composed of metal ions or clusters connected by organic linkers. These structures have gained significant attention in various fields due to their exceptional properties, including their importance in water adsorption. MOFs undergo a complex and lengthy process of maturation for scaling up and deployment, mainly due to the high cost of their precursors. Therefore, it is highly desirable to sustainably combine waste valorization and the use of waste materials as precursors to fabricate advanced porous solid-state materials. This study successfully demonstrates the preparation of Cr-terephthalate MOFs by combining metal salt and organic linker extracted from tannery effluent and waste plastic bottles. The waste from tanneries was used as the source of Cr(III), while terephthalic acid was obtained from the alkaline hydrolysis of plastic bottles. Appropriate extraction and assembly processes led to the functional Cr-MOFs, MIL-101(Cr) and MIL-53(Cr). The prepared MOFs showed similar properties (surface area, hydrolytic and thermal stability, and water adsorption performance) to similar MOFs synthesized from pure commercial-grade precursors, as confirmed by N2 sorption, XRD, TGA, and water adsorption experiments. The advancements made in this study represent significant progress in overcoming the bottleneck of MOF cost efficiency and pave the way for easy scaling-up and maturation of MOF-based processes.

Acknowledgements: This work was supported by Research and publication office of Wollo University (Ethiopia) and Mohammed VI Polytechnic University (UM6P) of Morocco

Keywords: Metal-Organic Frameworks, water adsorption, waste valorization

NanoRecVeg Platform: selection of plants genetic resources for nanoemulsions synthesis

A. G. Vieira[1], M. P. B. Martins[2], F. A Silva[2], C. C. Bonatto[3], T. M. Pereira and L. P. Silva[3].
1 Universidade de Brasília, Departamento de Genética e Morfologia, 70910-900, Brasília, Brazil; 2 Universidade de Brasília, Instituto de Biologia, 70910-900, Brasília, Brazil; 3 Embrapa Recursos Genéticos e Biotecnologia, Laboratório de Nanobiotecnologia, 70770-917, Brasília, Brazil; 4 Universidade de Brasília, Departamento de Biologia Celular, 70910-900, Brasília, Brazil.
alicegovieira@gmail.com

Oil-in-water (O/W) nanoemulsions are homogeneous systems, in which nanometric oil particles are dispersed in aqueous media, enabled by the use of surfactants [1]. Nanoemulsions find different purposes, such as in the pharmaceutical, cosmetic, food and agricultural industries. That said, the NanoRecVeg platform proposes to establish an extensive screening of plant genetic resources (PGR) with potential for the nanomaterials synthesis, among these, O/W nanoemulsions. The evaluated PGR were provided by the curators of the Active Germplasm Banks (AGBs) and Embrapa Collections. The first samples received were from AGB Cashew, provided from Fortaleza, Ceará, Brazil. The cashew seeds (*Anacardium occidentale*) were boiled, dried and grinded. The nuts oils were extracted using organic solvents, such as water, chloroform and methanol, and were incorporated into the aqueous solution of the green surfactant, soy lecithin. The produced nanoemulsions were characterized using dynamic light scattering and the main parameters evaluated were hydrodynamic diameter (HD), Zeta potential (ZP) and polydispersity index (PdI). Among the samples tested, the average HD related to intensity showed a minimum value at 189.9 ± 9.3 nm and a maximum value at 254.2 ± 23.3 nm. The particle size was satisfactory, remaining within the nanometer scale. The nanoemulsions showed the mean value of ZP between -23.6 ± 0.4 mV and -40.3 ± 2.9 mV, indicating that the formulated nanoemulsions had incipient to good colloidal stability. Finally, the PdI found varied between 0.33 ± 0.01 and 0.74 ± 0.04, which indicates the variability between moderately to slightly homogeneous nanoemulsions. Cashew seeds appear to have potencial for nanobiotechnological applications, more specifically, in the synthesis of nanoemulsions. It is expected that hundreds of O/W nanoemulsions will be synthesized and analyzed to compose a broad database, which will provide subsidies for the development of new products.

[1] J. C. Nunes et al., Influência da nanoemulsão de óleo essencial de limão em filmes à base de gelatina, Química Nova. 41, 1006 (2018).

Acknowledgements: This work was supported by CNPq and Embrapa Recursos genéticos e Biotecnologia.

Keywords: nanoemulsion; cashew oil; plant genetic resources; active germplasm banks;

Thermoplastic films of starch and polyvinyl alcohol with bacterial cellulose nanoreinforcements

Amanda de S. M. de Freitas[1], Marystela Ferreira[2], Maria Laura Foresti[3] and Ana Paula Lemes[1]
[1]Federal University of São Paulo, Institute of Science and Technology, 12231-280, São José do Campos, Brazil;
[2]Federal University of São Carlos, Science and Technology Center for Sustainability, 18052-780, Sorocaba, Brazil;
[3]University of Buenos Aires, Biotechnology and Biobased Materials Group, Buenos Aires, Argentina.
amandasq@hotmail.com

The production of nanocomposites from starch can be a sustainable strategy for the preparation of materials with biomedical applications[1]. Thus, the plastification of starch with glycerol and water allowed obtaining thermoplastic starch (TPS) and the subsequent preparation of a blend together with polyvinyl alcohol (PVA), in a ratio of 90:10 (m/m). Through the purification of bacterial cellulose (BC) membranes, nanofibrils (NFBC) were produced by basic hydrolysis[2]. The prepared reinforcements were used in the proportions of 2.5, 5.0 and 10.0% of NFBC. Thus, nanocomposite films of TPS/PVA/NFCB were produced in the established proportions. The produced nanocomposite films were characterized in terms of thickness, swelling and mechanical properties. The analyzes were carried out seeking to optimize and standardize the methodology to obtain materials with reproducible results that would allow the development of materials with possible application as transdermal dressings. The films presented a thickness within the desired range for application as a dressing, with an average thickness of 0.094 mm. Measurements of the swelling capacity of the films in phosphate buffer (pH 7.0) were also carried out. Based on this test, it was possible to observe that the addition of NFBC increased the swelling capacity of the films, in relation to the control, however, with the increase in the % of NFCB added, there was a reduction in the swelling capacity among the added samples. As for the mechanical properties, the Young's modulus increased as a greater amount of nanoreinforcement was added. As for the elongation at break, the incorporation of 2.5% NFCB increased the elongation capacity of the films, however the additions of higher percentages (5.0 and 10.0%) decreased the elongation capacity of the film. An increase in the maximum stress supported by the nanocomposite films can also be observed with the increase in the NFBC concentration, when compared to the sample without reinforcement. The best result for this property being obtained with the addition of 10% of NFBC, which led to an increase of approximately 10 times in the supported tension. Thus, the sample with 10% NFCB showed the desired thickness, swelling capacity and elongation for a promising application as a transdermal dressing[3].

[1] A. Das, S. Bhattacharyya, R. Uppaluri, C. Das, Int. J. Biol. Macromol. 2020, 155, 260.
[2] M.L. Cacicedo, M.C. Castro, I. Servetas, L. Bosnea, K. Boura, P. Tsafrakidou, A. Dima, A. Terpou, A. Koutinas, G.R. Castro, Bioresour. Technol. 2016, 213, 172.
[3] P.L. da Silva, A.M.M. Gomes, N.M.P.S. Ricardo, T.F. Machado, Quim. Nova 2016, 39, 450.

Acknowledgements: This work was supported by CAPES, grant 88882.430936/2019-01 (ASMF). FAPESP projects 2019/15976-0 (APL) and 2020/12659-0 (MF); CNPq grants 313989/2018-4 (APL) and 301955/2019-0 (MF). The authors would like to thank the universities involved and servier art image bank.

Keywords: Thermoplastic starch; polyvinyl alcohol; Bacterial Cellulose; Nanobiocomposites.

Magnetic flocculation of Chlorella sp. using Fe3O4 nanoparticles functionalized with tannin

Ana Carolina de Lima Barizão[1], J. P. Oliveira[2] and S. T. Cassini[1],
Federal University of Espírito Santo, Department of Environmental Engineering, LACAR, 29075-910, Vitória-ES; Brazil;
2 Federal University of Espírito Santo, Department of Morphology, NanoBio, 29053-360, Vitória-ES, Brazil.
ana.barizao@edu.ufes.br

Microalgae cultivation do not require arable lands and result in versatile biomass, applied to many kinds of biofuel [1]. However, their harvesting process is usually hard and costly [2]. In this way, this work aimed to optimize the biomass harvesting process of Chlorella sp., applying magnetic nanoparticles (MNPs) functionalized with tannin. Due to the high number of variables that can interfere in the harvesting process we i) realized a fractional factorial design ((2^{6-1}) microalgae concentration, MNPs concentration, pH, temperature, agitation, and contact time)) to identify the most significant variables in the system, using the harvesting efficiency (HE) as the response variable (680 nm); ii) variables that most interfered in the harvesting process were selected for optimization using a full factorial design (3^2). The produced MNPs presented a round shape and an average diameter of 11,50±2,65. The XDR analysis confirmed the magnetite crystalline phase, due to the characteristic peaks found at 30.10°, 35.46°, 45.54°, 56.6°, and 62.60°, which correspond to (220), (311), (400), (422), and (440). The FTIR demonstrated the range 3,000-3,500 cm-1 characteristic of hydrogen-bonded O-H, proving the formation of iron oxide. Peaks in 2,003 cm-1, were related to the N-CH2 stretching of third amines; 1,280 cm-1and 1,057 cm-1 were related to the C-O stretching of phenolic compounds [3]. The functionalized MNPs became more positive, going from -11 mV to 13 mV zeta potential (pH=4). In the fractional factorial, the pH and MNPs concentration were the most influential and selected for full factorial. The variable that most interfered with the system was pH ($p<0.05$) with an optimum value of 4.0. For the concentration of MNPs, the optimum value was 1,000 mg. L^{-1}, achieving a HE=92.6% and a q_{exp}= 1.39 g. mg-1. This could occur due to the protonation of the amino groups present in the tannin structure, making its surface charge positive (from -10 mV at pH=10 for +13 mV at pH=4), increasing attraction between MNPs and the negatively charged microalgae, favoring flocculation. The validation of the model (R2=0.96) was proven by performing the experiments under optimal conditions; resulting in a HE%= 95% higher than theoretical HE%= 92.6%. Thus, it was possible to conclude that the proposed method is highly efficient in harvesting microalgae biomass.

[1] C. Estudillo-del Castillo, E.M. Ligot, L.P. Nudo, Growth performance and lipid profiles of some tropical microalgae: An assessment of their potential as biofuel source, Biocatal Agric Biotechnol. 50 (2023) 102699. https://doi.org/10.1016/J.BCAB.2023.102699.
[2] J. Kim, G. Yoo, H. Lee, J. Lim, K. Kim, C.W. Kim, M.S. Park, J.W. Yang, Methods of downstream processing for the production of biodiesel from microalgae, Biotechnol Adv. 31 (2013) 862–876. https://doi.org/10.1016/J.BIOTECHADV.2013.04.006.
[3] B. Stuart, Infrared Spectroscopy_ Fundamentals and Applications, 2004.
Acknowledgements: This work was supported by Coordination of Improvement of Higher-Level Personnel (CAPES) The authors would like to thank team of researchers LACAR Laboratory.
Keywords: microalgae, iron oxide, harvesting.

Effect of nitric oxide-releasing nanoparticles on soybean seeds

Ana Cristina Preisler[1], Ana Luisa de Oliveira Simões[1], Juliana de Carvalho Izidoro[2], André Luiz Floriano Jacob[2], Amedea Barozzi Seabra[2], Halley Caixeta de Oliveira[1]
1 State University of Londrina, PR 445, km 380, 86057-970 Londrina, PR, Brazil;
2 Federal University of ABC
(UFABC), Santo André, SP, Brazil.
preislerac@gmail.com

Nitric oxide (NO) is a small and gaseous molecule that participates in several processes of plant growth and development, like germination, in addition to acting in defense against stress [1]. The exogenous application of NO in plants requires the use of NO donors, such as S-nitrosoglutathione (GSNO). However, these compounds present relative instability and are susceptible to degradation.Thus, the use of nanocarriers appears as a promising alternative for the application of NO donors in agriculture [2]. However, there is still a gap related to the interaction mechanisms between nanomaterials and plants. Therefore, the objective of this study has been to evaluate and compare the effects of free and nanoencapsulated GSNO using nanoparticles with different compositions and charges on germination and initial growth of soybean seedlings. The experiment was conducted in a germinator for eigth days, under a controlled temperature of 25 ºC, relative humidity of 95 ± 1% and photoperiod of 12 h using seeds of Glycine max L. Merr. (BRS 257). The treatments were control (distilled water), chitosan nanoparticles (NP CS) with and without GSNO, alginate nanoparticles (NP Al) with and without GSNO, and free GSNO. For each treatment, there were four biological replicates with 50 seeds each. The concentrations of the formulations were 0 mM (control), 0.125 mM, 0.250 mM, 0.500 mM, 1.0 mM, and 2.0 mM. Seed treatment was by imbibition with 100 mL of the formulations for 5 minutes. Seed germination and morphological parameters were evaluated eight days after the treatment. For the percentage of germination, the differences were significant for NP CS with and without GSNO, and free GSNO, so the data were adjusted by polynomial regression. For the NP AL-GSNO, it was not possible to adjust, but we observed an increase of 16%, 11%, and 14%, respectively, for the concentrations 0.125, 1.0, and 2.0 mM compared to the control. An interesting data was that the concentration of 1 mM NP CS showed higher values of germination compared to the formulation containing GSNO. Overall, the 2.0 mM concentration reduced the germination rate, except for the NP Al formulation. The number of secondary roots (NSR) gradually increased for the NP CS-GSNO, NP Al-GSNO, and free GSNO formulations. For NP Al-GSNO, the NSR was approximately three times higher in the highest concentrations. On the other hand, for shoot and root length NP Al-GSNO showed no significant effect. As for NSR, NP CS-GSNO showed negative effects on root and shoot length. Free GSNO showed a positive effect for the root, but not for the shoot. NP CS-GSNO increased the root dry mass while NP AL-GSNO increased the shoot dry massa. The different induced effects may be related to the different characteristics of the formulations and how they alter the bioavailability of NO in the plant. Therefore, more detailed studies are still needed to elucidate this interaction.

[1] Su-Ee. Lau, M. F. Hamdan, Teen-Lee. Pua, N. B. Saidi, B. Chin Tan, Plant nitric oxide signaling under drought stress. Plants. 10, 2, 360 (2021)
[2] A. B. Seabra et al. Nitric oxide-releasing nanomaterials: from basic research to potential biotechnological applications in agriculture. New Phytologist, 234, 4, 1119-1125 (2022)
Acknowledgements: The present work was carried out with the support of the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brazil (CAPES) – Process 001, FAPESP and CNPq.

Evaluation of the effects of nanoatrazine bioconcentration on the aquatic trophic chain in phytoplankton, zooplankton, and fish

Ana Paula Andrade Braga[1], Vera Lucia Scherholz Salgado de Castro[2], Leonardo Fernandes Fraceto[3]
1 São Paulo State University (UNESP), Department of Biology, 13506-900, Rio Claro, Brazil; 2 Embrapa Environment, Laboratory of Ecotoxicology and Biosafety, 13918-110, Jaguariúna, Brazil; 3 São Paulo State University (UNESP), Environmental Nanotechnology Laboratory, Sorocaba, Brazil.
apandradebraga@gmail.com

Atrazine is a widely used herbicide in Brazil, known for its persistence in aquatic environments. however, its leaching potential and absorption by organic matter have led to the accumulation of the herbicide in soils and water bodies, raising concerns about potential ecotoxicological effects occurrence[1]. In this sense, the nanoencapsulation of the herbicide atrazine can be a suitable strategy to minimize adverse effects in agriculture in comparison to its commercial formulation[2]. The nanoatrazine (nATZ) efficiency studies in target species have shown high efficacy in weed control, even at concentrations ten times lower than those recommended for conventional formulation[3]. However, while there is evidence regarding the efficiency of nATZ, the knowledge about the toxicological effects of its application is still limited, and safe concentrations for exposure in non-target organisms are still unknown[4]. Besides, the rapid development of nanopesticides raises concerns about their possible health risks as oxidative stress and environmental impacts, including the potential to be transferred into food chains[5, 6]. To gain a better understanding of this issue, a freshwater food chain consisting of three trophic levels will be studied. Representative organisms from each trophic level, including algae, microcrustaceans and fish, will be evaluated for the effects of bioconcentration and biomagnification of nATZ using polycaprolactone polymer (nATZ-PCL). Initially, the algae species Raphidocelis subcapitata (primary producer) will be exposed to different concentrations of nATZ-PCL. Next, neonates of Daphnia magna (primary consumers) will be fed with the pre-exposed algae, and subsequently, they will serve as prey for Danio rerio fish (secondary consumers). After the exposure period, the quantification and assessment of the ecotoxic effects of nATZ on the exposed organisms will be conducted. In addition, biochemical analyses, including the enzymatic activity of antioxidant enzymes (catalase, superoxide dismutase, and glutathione S-transferase), will be performed. This study aims to expand the understanding of the ecotoxicological effects of nATZ-PCL along the aquatic food chain and develop a protocol for this type of evaluation. The research results are expected to contribute to the development of safer nanopesticides that reduce negative impacts on the environment and public health.

[1] S. Rostami. et al. Atrazine exposed phytoplankton causes the production of non-viable offspring on Daphnia magna. Marine Environmental Research, v. 145, n. February, p. 177–183 (2019).
[2] F. P. De Albuquerque. et al. Use of nontarget organism Chironomus sancticaroli to study the toxic effects of nanoatrazine. Ecotoxicology, v. 30, n. 4, p. 733–750 (2021).
[3] G. Tortella. et al. Nanoparticles as a Promising Strategy to Mitigate Biotic Stress in Agriculture. Antibiotics, v. 12, n. 2 (2023).
[4] T. B. Hennig. et al. A systematic review of the toxic effects of a nanopesticide on non-target organisms: Estimation of protective concentrations using a species sensitivity distribution (SSD) approach – The case of atrazine. Science of the Total Environment, v. 871 (2023).
[5] E. Martinez, L. Alves. Interaction of nanomaterials with biosystems and the nanotoxicology: in the direction of regulation. Journal of the Brazilian Society for the Advancement of Science, v. 65, p. 32–36 (2013).
[6] M. Chen. et al. Interaction of nanomaterials with biosystems and the nanotoxicology: in the direction of regulation.

Journal of the Brazilian Society for the Advancement of Science, v. 65, p. 32–36 (2013).
Keywords: ATZ nanoparticle, nanotoxicology, trophic transfer

Development of Solid Lipid Nanoparticles incorporating bioactive coumarin analogues as photosensitizing agents

A. Katopodi[1,2], K. Safari[1], A. Kalospyros[1,2], K. Politopoulos[2], E. Alexandratou[2] and A. Detsi[1*]
1 Laboratory of Organic Chemistry, School of Chemical Engineering, National Technical University of Athens, Zografou, Campus, Athens, Greece,; 2 Laboratory of Biomedical Optics and Applied Biophysics, School of Electrical and Computer Engineering, National Technical University of Athens, Zografou Campus, 15780 Athens, Greece
**adetsi@chemeng.ntua.gr*

Coumarins are a family of heterocyclic compounds which possess a wide range of biological activities, such as antioxidant, anti-inflammatory, anticancer and neuroprotective. Daphnetin (7,8-dihydroxy-coumarin), is a naturally occurring coumarin, isolated from plants of the genus *Daphne* and distinguished for its significant therapeutic profile. However, daphnetin can be susceptible to air or light oxidation due to the catecholic moiety. In this context, we present herein the encapsulation of daphnetin and its synthetic analogue, 7,8-dihydroxy-3-(4-hydroxyphenyl)-4-methyl-coumarin, in Solid Lipid Nanoparticles (SLNs), as well as the evaluation of their biological activities. The SLNs were formed using the emulsification solvent-evaporation method combined with ultrasonication. The SLNs were characterized using Dynamic Light Scattering, FT-IR spectroscopy and Thermogravimetric Analysis methods. The coumarin analogues and their SLNs formulations were evaluated for their antioxidant activity via evaluation of (i) their ability to scavenge the stable free radical DPPH and (ii) their ability to inhibit lipid peroxidation. It is noteworthy that the coumarin loaded SLNs exhibited improved antioxidant activity than the coumarin analogues in their free form possibly due to a synergistic effect between the lipid components and the coumarins. The optical properties, stability and Reactive Oxygen Species production ability, as well as the ability of the coumarins and the corresponding SLNs to act as photosensitizers against A431 epidermoid carcinoma cell line were also studied. Both coumarin analogues presented phototoxic activity, while 7,8-dihydroxy-3-(4-hydroxyphenyl)-4-methyl-coumarin exhibited significant PDT activity both in its free and encapsulated form, consisting a promising theranostic agent.

[1] A. Katopodi, E. Tsotsou, T. Iliou, G.E. Deligiannidou, E. Pontiki, C. Kontogiorgis, F. Tsopelas, A. Detsi, Molecules 2021, 26, 5999.
[2] A. Katopodi, A. Detsi, Colloids and Surfaces A: Physicochemical and Engineering Aspects 2021, 630, 127529.
[3] E. Kavetsou, C. Tsoukalas-Koulas, A. Katopodi, A. Kalospyros, E. Alexandratou, A. Detsi, Bioengineering, 10(2), 244.

Acknowledgements: A. K. gratefully acknowledges State Scholarships Foundation (IKY). This research is co-financed by Greece and the European Union (ESF) through the Operational Programme (Human Resources Development, Education and Lifelong Learning) in the context of the project “Strengthening Human Resources Research Potential via Doctorate Research” (MIS-5000432), implemented by the State Scholarships Foundation (IKY).

Keywords: coumarins, Solid Lipid Nanoparticles, Photodynamic Therapy

Characterization and migration studies of PLA multilayer film functionalized with cellulose nanocrystals and chitosan

Antía Lestido-Cardama[1,2], Miguel Cerqueira[1], Lorenzo Pastrana[1] and Ana Isabel Bourbon[2]
[1] *INL, International Iberian Nanotechnology Laboratory, Av. Mestre José Veiga s/n, Braga, Portugal*
[2] *University of Santiago de Compostela, Department of Analytical Chemistry, Nutrition and Food Science, Faculty of Pharmacy, Campus Vida, Santiago de Compostela, Spain*
antia.lestido@inl.int

Food packaging has become an essential tool in food manufacturing since it protects them against contamination, preserving their nutritional and sensory properties, and extending the product's shelf life. Nowadays, there has been a marked increase in the use of biopolymer-based active packaging film, which can improve the shelf life of food. Polylactic acid (PLA) is one of the most attractive bio-based polymers used for food packaging due to its good properties. However, its use has been limited because of the poor barrier properties, high brittleness, low toughness, slow crystallization rate and low thermal stability. One of the strategies to improve the active and barrier properties of PLA is the application of coating technology. Nevertheless, the impact of these active additives into foodstuff and on consumer' health still be unknown. In the present study, alternating layers of cellulose nanocrystals (CNC) and chitosan were applied on PLA film using the spray coating technique. Physicochemical characterization of the nanoparticles and the film was carried out by combining various techniques. The migration of CNC applied in the packaging material to food were carried out according to European Normative. Specific migration of CNC from films has been tested by immersion of the side of film with multilayer system in three food simulants at 40 °C during 10 days. The quantification was carried out by calcofluor white fluorescence staining and by a colorimetric method for the determination of sugars. Microscopy techniques made it possible to visualize the needle-like shaped crystalline nanoparticles. The migration results obtained show that there is a small migration of the CNC from the coating ranging from 0.03 mg/L (isooctane) to 1 mg/L (3% acetic acid, v/v).

Acknowledgements: Antía Lestido-Cardama is beneficiary of a Margarita Salas contract funded by the Programme for requalification, international mobility and tlent attraction in the Spanish university system (grant UP2021-042). Ana Isabel Bourbon acknowledges funding by FCT, through the individual scientific employment program contract (2020.03447.CEECIND).

Keywords: biopolymer, cellulose nanocrystals, migration, polylactic acid

Mycosynthesis of Silver Nanoparticles (AgNPs) via Aqueous Extracts of Wild Mushroom (*Daedalea sp*.): Characterization, Environmental and biological investigation

Asif Kamal[1], Malka Saba[1]
[1]*Department of Plant Sciences, Quaid-i-Azam University Islamabad, 45320 Pakistan.*
kamal@bs.qau.edu.pk

The current study was carried out to synthesize silver nanoparticles (AgNPs) via green reduction method from a wild mushroom collected from Quaid-i-Azam University, Islamabad, Pakistan. The collected fungus was identified as *Daedalea sp.* based on morphological characteristics Wild mushroom, *Daedalea sp*. belong to division Basidiomycota and class agaricomycetes. *Daedalea species* used in bioremediation has been studied by several research groups. A number of harmful dyes and pigments have been shown to degrade when exposed to the lignin-degrading enzyme laccase, as isolated and purified from *Daedalea*. Horses with sensitive skin have been brushed down using the fruit bodies of *Daedalea sp*. and, therefore, the mushroom is considered as natural comb. The metallic oxide NPs based on *Daedalea* have much economic importance due to which they can be used for biomedical treatments of diseases and different agents like anti-cancer. *Daedalea* is a healthy fresh food cultivated on organic substrates and grown naturally in Pakistan and worldwide Myconanotechnology is a recently emerged field that describes the biosynthetic pathway of metallic and non-metallic NPs via reduction through various organic mycomaterials present in fungi for example, mushroom, yeast, and mold etc. for various applications, particularly, in biomedical field. Wild mushroom (*Daedalea sp*.) was used as an effective chelating agent for the mycosynthesis of silver nanoparticles (Ag-NPs) and significantly characterized through XRD, FTIR, energy dispersive spectroscopy and SEM/TEM. Antifungal assays against five human pathogenic fungal strains were carried out, and minimum inhibitory concentrations were calculated. Mucor species (FCBP 300) was the most susceptible strain to mycosynthesized AgNPs. All the fungal strains showed susceptibility to the Ag-NPs. MTT cytotoxic assay was carried out against the promastigote and amastigote cultures of Leishmania tropica and their IC50 values were calculated as 248 and 251 µg/mL. In brief, the negligible hemolytic activity against human RBCs at the highest concentration (400 µg/mL), as well as moderate antioxidant activities at low concentrations suggest the application of the fabricated Ag-NPs in environmentally sound and viable hygiene production. The photocatalytic activity of mycosynthesized Ag-NPs resulted in 98.2% degradation of indigo carmine dye in 140 minutes. *Daedalea sp* Ag-NPs can be used as novel candidates for a variety of biomedical and environmental applications due to their eco-friendly synthesis, biosafe nature, and excellent physicochemical properties.

Acknowledgements: National Center for Physics (NCP), Islamabad, is gratefully acknowledged for providing XRD, and FTIR facilities for sample characterization.

Keywords: Daedalea sp, Mycosynthesis, Silver nanoparticles, characterization

Detection of organic pollutants in water by surface-enhanced Raman spectroscopy

Ayelén A. Arias[1], Ana M. Hernández-Giménez[2], Judith Langer[2], Luis M. Liz-Marzan[2], and M. Fernanda Cardinal[1,2].

[1]*Instituto de Nanosistemas, Universidad Nacional de San Martín-CONICET, Av. 25 de Mayo 1021,1650, Buenos Aires, Argentina.*

[2] *CICbiomaGUNE, Paseo de Miramon 182, 20014, Donostia, San Sebastian, Spain.*

aarias@unsam.edu.ar

Argentina hosts the second-largest reservoir of unconventional oil and gas globally, primarily concentrated in the Vaca Muerta field [1]. In hydraulic fracturing, BTEX compounds (Benzene, Toluene, Ethylbenzene, and Xylenes) are commonly used as additives in stimulation fluids to enhance the production of unconventional oil and gas. These compounds also occur naturally in crude oil [2]. Phthalate esters (PAEs) are chemical compounds derived from oil and extensively employed as plasticizers to enhance the flexibility and durability of various plastic products. Due to their non-covalent bonding, PAEs can be easily released into the environment, acting as endocrine-disrupting compounds [3]. All of these substances pose risks to human health and the environment and can be found in contaminated surface and groundwater. The primary objective of our work is to develop a platform with suitable properties to detect organic industrial pollutants at very low concentrations by surface-enhanced Raman spectroscopy (SERS). Specifically, BTEX (toluene) and PAES (dimethyl phthalate, DMP) are our targeted molecules. The methodology employed involves several steps: first, the synthesis of citrate-capped gold spheres [4]; second, the functionalization of glass slides with an amino silane to facilitate the electrostatic attachment and growth of nanoparticles [5]; next, if necessary, surface modification; and finally, SERS measurements. Electron microscopy and UV-visible spectroscopy are typically utilized for sample characterization. Our preliminary results demonstrate that appropriately sized gold spheres, when attached and grown, can effectively detect the targeted molecules. Utilizing a portable macro Raman set-up, SERS substrates were studied using benzenethiol (BZT) as a probe molecule, revealing a significantly higher response signal for grown particles compared to non-grown spheres. Additionally, due to the lack of affinity between phthalates and metallic nanoparticles, surface functionalization of the particles was necessary to enable their capture and detection via SERS. In this regard, we investigated various self-assembled monolayers (SAMs) of alkanethiols and identified a suitable SAM for sensing DMP [6], achieving a detectable concentration value of 100 μM.

[1] L. Mastronardi. Unconventional hydrocarbons: The rise of Vaca Muerta. Ministerio de Hacienda, Argentina, (2019).
[2] F. Leusch & M. Bartkow. A short primer on benzene, toluene, ethylbenzene and xylenes (BTEX) in the environment and in hydraulic fracturing fluids. Griffith University, (2010).
[3] M. Palacios-Arreola. Environmental pollutants: an immunoendocrine perspective on phthalates. Frontiers in Bioscience, Landmark, 26, (2021), p 401-430.
[4] N. G. Bastús, J. Comenge, & V. F. Puntes. Kinetically Controlled Seeded Growth Synthesis of Citrate-Stabilized Gold Nanoparticles of up to 200 nm: Size Focusing versus Ostwald Ripening. Langmuir, 27, (2011), p 11098–11105.
[5] A.M. Fales, H.Yuan, & T.Vo-Dinh. Development of hybrid Silver-Coated Gold Nanostars for Nonaggregated Surface-Enhanced Raman Scattering. The Journal of Physical Chemistry C, 118, 7, (2014), p 3708-3715.
[6] Q. Zhang, W. Guo, L. He, L. He, Y. Chen, X. Shen, & D. Wu. A new SERS substrate of self-assembled monolayer film of gold nanoparticles on silicon wafer for the rapid detection of polycyclic aromatic hydrocarbons. Materials Chemistry and Physics, 250, (2020), 122994.
Acknowledgements: This work was financially supported by CONICET, CICbiomaGUNE Agencia I+D+i, and INS-UNSAM. *Keywords*: SERS, gold, phthalates, pollutants.

Pushing the Limits of Traditional Fertilizers: Nanofertilizers, Effective Nutrient Release Systems

Ojaimi, B. S.[1], Galembeck, A.[2] And Moreno, Y. P.[2]
1 Universidade Federal de Pernambuco, Departamento de Engenharia Química, 50740-540, Recife, Brazil;
2 Universidade Federal de Pernambuco, Departamento de Química Fundamental, 50740-560, Recife, Brazil.
Beatriz.ojaimi@ufpe.br

Faced with the growing pressure exerted on the agricultural sector to meet future demands for food and provide food security for the population that is constantly expanding, the perception of the need to develop new methods to drive modern precision agriculture.1 In this context, a strategy aimed at the sustainable intensification of agriculture is based on the use of technologies that have a sparing effect on scarce resources, given the limited availability of land and water resources.2 In terms of plant nutrition, a crucial step in crop productivity, the use of chemical fertilizers is a pillar of any agricultural economy. However, there are several problems associated with the use of conventional fertilizers, including environmental threats and their efficiency in terms of nutrient delivery. Thus, with the extensive innovation action in this field, there is the emerging advent of nanotechnology applied to agriculture, which provides tools with high potential to improve the efficiency of the process of meeting the nutritional needs of crops. The use of nanofertilizers stimulates productivity, with the greater efficiency of these products due to their low toxicity, high mobility and, mainly, their reduced size, due to the increased surface area.3 Considering this, this work seeks to evaluate the efficiency of formulated silica nanoparticles as carriers of the macronutrients NPK. The synthesis of NPs was carried out using the Stöber methodology, using solutions of KH2PO4, KNO3 and CH4N2O as nutrient precursors for their encapsulation in the nanoparticle matrix. Four suspensions were prepared, including the control, two prepared with the use of precursors, one of them with the presence of chitosan, and one that was incorporated with a commercial fertilizer. The analysis of the morphology of the particles was performed using SEM and TEM. Characterizations were carried out to evaluate the hydrodynamic diameter through the DLS technique, surface charge through the ZP, and specific surface area, through Nitrogen Porosimetry using the BET method. To verify the levels of nutrients that were incorporated, the Kjeldahl method was used to determine nitrogen, and ICP-OES to quantify phosphorus and potassium. Also, a leaching test was carried out to study the release of nutrients into the medium according to time. Through the studies, it was possible to conclude that the produced nanoparticles are small enough in size to not find great restrictions to be absorbed by the plant, with average diameters ranging from 39,21 to 785,11 nm. From the results obtained, it was possible to prove that the synthesis of mesoporous silica nanoparticles allowed the incorporation of NPK macronutrients.

[1] Murgueitio-Herrera, E., Falconí, C., Cumbal, L., Gómez, J., Yanchatipán, K., Tapia, A., Martínez, K., Sinde-Gonzalez, I. and Toulkeridis, T. Synthesis of Iron, Zinc, and Manganese Nanofertilizers, Using Andean Blueberry Extract, and Their Effect in the Growth of Cabbage and Lupin Plants (Nanomaterials, 2022).
[2] Vieira Filho, J. Expansion of the agricultural frontier in Brazil: challenges and perspectives. (IPEA, 2016).
[3] Sasson, Y., Levy-Ruso, G., Toledano, O. and Ishaaya, I. Nanosuspensions: emerging novel agrochemical formulations (Springer Berlin Heidelberg, 2007).

Acknowledgements: This work was supported by the Fundação de Amparo à Ciência e Tecnologia de Pernambuco. The authors would like to thank the support of the institutions that allowed the development of the research and the opportunities to stimulate it.

Keywords: Stöber Silica, Precision Agriculture, Nanofertilizers.

Metribuzin nanoformulation safety assessment in soil non-target organism

Brian Cintra Cardoso[1], Vanessa Takeshita[1], Gustavo Vinicios Munhoz-Garcia[1], Camila Werk Pinácio[1], Leonardo Fernandes Fraceto[2], Valdemar Luiz Tornisielo[1]

Center of Nuclear Energy in Agriculture, University of São Paulo, Piracicaba, Brazil[1], Science and Technology Institute, State University of São Paulo, Sorocaba, Brazil[2]

brianccardoso@usp.br

The minimization of environmental impacts has been an essential stimulus for developing sustainable technologies, especially in agriculture, given the widespread use of pesticides for crop protection. In this sense, nanoformulations may be allies capable of reducing the negative effects caused by the dissipation of pesticides, with the help of a controlled release and small doses when compared to those conventionally used. This research aimed to evaluate the effects of a biodegradable nanoformulation for the herbicide metribuzin on soil bioindicator organisms (*Eisenia andrei*). Starting with an acute test, earthworms were exposed for 14 days to nanoformulation of metribuzin (based on poly-ε-caprolactone) and the commercial formulation of the product. The experimental units consisted of 750 mL jars containing 500 g of soil and 10 organisms. A range of 5 doses was used for the evaluation of the acute effects of the formulations (120,240,480,960,1920 g.i.a ha-1). No lethality effects of the earthworms were observed within the studied period at any of the tested doses, in addition, there was no significant loss of mass of the organisms (361 mg) compared to the control soil without herbicide application (338 mg) at the highest dose tested, evidencing the safety of the nanoformulation. In addition, the earthworms exposed to nanoformulation showed a greater vigorous response to mechanical stimuli. The results indicate that the nanoformulation is safe for the organisms, even at the highest dose. Further studies are needed to verify chronic and biological effects on the tested organisms, aiding in the validation of new, safer formulations for application to crops.

Acknowledgements: This work was supported by São Paulo Research Foundation (Process #2022/01554-9; #2021/03455-5; #2019/04758-1; #2022/00509-0; #2022/00718-8, #2017/21004-5).

Keywords: nanoparticles, environmental risk, non-target organisms, ecotoxicology.

Evaluation of the clinical safety of nano-encapsulated cloxacillin benzathine for treating caseous lymphadenitis in goats

Soares, B C F[1]; Felix, L A[1]; Gonzaga, L W F[1]; De Almeida, J V F C[1]; Faccioli-Martins, P Y[2]; Corrêa, D S[3]; Ferrante, M[1]; Brandão, H De M[4]

[1]*College of Animal Science and Veterinary Medicine (FZMV), Federal University of Lavras (UFLA), Lavras, Minas Gerais, Brazil.*

[2]*Brazilian Agricultural Research Corporation (Embrapa) Goats and Sheep Unity, Sobral, Ceará, Brazil.*

[3]*Embrapa Instrumentation Unity, São Carlos, São Paulo, Brazil.*

[4]*Embrapa Dairy Cattle Unity, Juiz de Fora, Minas Gerais, Brazil.*

e-mail: humberto.brandao@embrapa.br

The use of nanostructured antibiotics can contribute to therapeutic efficacy and microbiological cure, as demonstrated in previous studies by our team using nano-encapsulated benzathine cloxacillin (patent WO/2011/150481) against *Staphylococcus aureus* and *Moraxella bovis* in bovine mastitis [1] and infectious keratoconjunctivitis [2], respectively. Cloxacillin nanoparticles exhibited sizes of 188.41 ± 49.34 nm, polydispersity index of 0.181 ± 0.07, and Zeta potential of -33.93 ± 6.42 mV. During the development process of a new drug, evaluation of the pharmacological safety profile is necessary. This work aims to evaluate the clinical safety of using cloxacillin-loaded polymeric nanospheres (CLXNP) in treating caseous lymphadenitis in goats by the subcutaneous (SC) peri-abscess route. Eight Toggenburg females, weighing 30 to 52 kg and aged between nine months to three years, naturally infected with *Corynebacterium pseudotuberculosis*, received 1.81 mg/kg of CLXNP by the SC peri-abscess route. A veterinarian clinically evaluated each animal and measured various physiological parameters such as body temperature, heart rate (HR), respiratory rate (RR), pain during palpation, and other adverse reactions at the application site, as well as measuring lymph nodes and collecting blood samples. The animals did not demonstrate local or systemic clinical manifestations, such as edema in the application region, pain on palpation, fever, or increased HR or RR, which would be consistent with adverse reactions to antibiotic therapy. In addition, they did not stop eating or show discomfort when moving around. Thus, this preliminary data can guide a more extensive clinical study in goats infected with *C. pseudotuberculosis* to define an initial dose for the species and a reasonable interval between doses for treating caseous lymphadenitis with CLXNP.

[1] ARAÚJO, R. S.; GARCIA, G. M.; VILELA, J. M. C.; ANDRADE, M. S.; OLIVEIRA, L. A. M.; KANO, E. K.; LANGE, C. C.; BRITO, M. A. V. P. E.; BRANDÃO, H. M.; MOSQUEIRA, V. C. F. Cloxacillin benzathine-loaded polymeric nanocapsules: Physicochemical characterization, cell uptake, and intramammary antimicrobial effect. Materials Science & Engineering: C - Materials for Biological Applications, v. 104, p. 110006, 2019. doi:10.1016/j.msec.2019.110006.

[2] FONSECA, M. D. M., MAIA, J. M. S., VARAGO, F. C., GERN, J. C., CARVALHO, W. A., SILVA, S. R., MOSQUEIRA, V. C. F., BRANDÃO, H. M., & GUIMARÃES, A. S. Cloxacillin nanostructured formulation for the treatment of bovine keratoconjunctivitis. Veterinary and Animal Science, 9, 100089. 2020. https://doi.org/10.1016/j.vas.2020.100089

Acknowledgments: We conduct this research in partnership with EMBRAPA Goats & Sheep, Instrumentation, and Dairy Cattle Unities. It was funded by EMBRAPA (SEG20.20.03.002.00.00), Funcap (BP5-0197-00148.01.00/22), FAPEMIG (APQ-01168-21), CAPES (88887.805529/2023-00), and CNPq (448011/2014-0).

Keywords: goats; nanotechnology; antibiotic therapy; clinical safety.

Synthesis and Characterization of Chitosan-Based Nanofertilizers

Camilla Emanuella Borba Pereira[1φ], Yolice Moreno Ruiz[2], André Galembeck[3], Valesca Pandolfi[1]
[1] *Universidade Federal de Pernambuco, Departamento de Genetíca, 50670-423, Recife, Brazil;*
[2] *Universidade Federal de Pernambuco, Centro Acadêmico de Vitória, 55608-680, Vitória de Santo Antão, Brazil;*
[3] *Universidade Federal de Pernambuco, Departamento de Química Fundamental, 50740-600, Recife, Brazil*
camilla.borba@ufpe.br

Brazil is one of the largest exporters of agricultural products worldwide and plays an essential role in global food production. However, it is ranked first on the list of fertilizers importing countries in 2022, spending almost USD 25 billion [1]. Fertilizers supply the essential nutrient for plant growth, thus increasing crop yield [2]. On the other hand, the overuse of chemical fertilizers is an emerging concern due to significant losses during their application. After all, about 40-70% of nitrogen, 80-90% of phosphorus, and 50-90% of potassium are wasted [3]. As a result, several environmental damages, such as eutrophication, and soil compaction, are triggered. Among the strategies to overcome these problems, nanotechnology is being considered to develop controlled and slow release of nutrients improving nutrient uptake and reducing their environmental impact [4]. This work aimed to develop a chitosan-based nanofertilizer loaded with N, P, and K. Plants of *Arabidopsis thaliana* and *Eruca sativa* were selected on behalf of their short life cycle and economic relevance, respectively. Chitosan was chosen as the primary material due to the promising results of previous tests carried out on sugarcane crops by our research group. Nanoparticles were obtained using microfluidic technology through the ionotropic gelation [5] by the interaction between chitosan and sodium tripolyphosphate (TPP). Macronutrient solutions with KNO3, CH4N2O, and KH2PO4 were used at four levels of nutrient loads, following pre-established concentrations. The incorporation was made through the addition of these solutions during the synthesis. The hydrodynamic diameter was analyzed through Dynamic Light Scattering, NPs presented average sizes ranging from 960 to 1400 nm. Zeta Potential was used to determine the surface charge of the NPs and stability. Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM) were used to analyze nanoparticle size, morphology, and structure and to ensure that the NPs are small enough to enter an ostiole. Macronutrient concentrations (K and P) incorporated into nanoparticles were quantified by Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). Thermogravimetric analysis (TGA) was carried out to evaluate thermal stability. Results obtained so far showed that the NPs are loaded with N, P, and K and they are small enough to enter the ostiole and deliver nutrients to plants.

[1] Statista, Leading Fertilizer Importing Countries Worldwide in 2022 Based on Value, 2023.
[2] H. Reetz, Fertilizers and Their Efficient Use (International Fertilizer Industry Association) 2016.
[3] P. Solanki, H. Chippa, et al., Nano-fertilizers and Their Smart Delivery System (Nanotechnology in food and agriculture) 2015.
[4] S.K. Saha, S.M.A. Rahman, et al., Nanofertlizers-A Potential Alternative to Chemical Fertilizers, 2 (2021), p 32-37.
[5] P. Calvo, C. Remuñán-Lópezet al., Novel hydrophilic chitosan-polyethylene oxide nanoparticles as protein carriers (Jounal of Applied Polymer Science) 1997.

Acknowledgments: This work was supported by Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES). The authors would like to thank the Programa de Pós-Graduação em Ciências Biológicas, UFPE.

Keywords: nanofertilizers, Eruca sativa, Arabidopsis thaliana, and synthesis.

Aquatic ecotoxicological evaluation of water sampled with exhaust gases from burning different fuel mixtures containing S10 diesel, 1G ethanol, 2G ethanol, and HVO, using *Daphnia Similis* as test organisms

Clara Rodrigues Pereira[1], Eliete C. Alves[1], Adriano Carvalho Simões Guimarães[1], Edna dos Santos Almeida[1] and Lilian Lefol Nani Guarieiro[1]

[1] Centro Universitário SENAI CIMATEC; Salvador, Bahia, Brazil.

clara.r.pereira@gmail.com

The contamination of aquatic environments by fuels is increasingly in evidence due to the composition of fuels having the presence of polycyclic aromatic hydrocarbons of a toxic and carcinogenic nature [1,2]. In this context, PAHs can be formed from the incomplete combustion of fuels, such as petroleum derivatives and refined products, and these substances can accumulate in sediments, aquatic organisms, and the water column, in low concentration [2]. In this way, alternative fuels such as natural gas, hydrogen, ethanol, butanol, and biofuels are considered possible substitutes, since they can promote better efficiency in their combustion, performance, and emissions [3]. In this context, methodologies for analyzing the toxicity of the implementation of methods of this nature can be considered for the evaluation of this aqueous medium or effluent, resulting from this process. Among the toxicity tests, acute ecotoxicity stands out, since daphnia are the main bioindicators used to assess the toxicology of water quality, so they have species, such as Daphnia Similis that can be found both in the sea and in freshwater, and are constantly applied in ecotoxicity tests [4]. Thus, in view of the information presented, this study aims to evaluate the toxicity of water sampled with gases from the burning of different fuel mixtures, using Daphnia Similis. The methodology consisted of a diesel cycle engine with a fixed speed of 1500rpm (4 cylinders, continuous power 82CV, 66KVA, intermittent power 90CV, 73KVA, and turbo aspiration) mounted under a stationary dynamometer (AVL with the capacity to absorb up to 240 kW). The fuels used for this experiment consisted of the following mixtures: Diesel S10 Pure; diesel S10 with 10% ethanol 1G (S10E1G); diesel S10 with 10% ethanol 2G (S10E2G); S10 diesel with 10% HVO (S10HVO). The system consisted of two bubblers in series (Impingers), adapted from the NBR 12026 standard. The results showed an increase in mortality when analyzing the culture solution with pure S10 exhaust gases, considering that with the addition of 1G ethanol to diesel, there was a reduction in the mortality of organisms, in the same way, that for the mixture of S10 diesel with 2G Ethanol, there was an even greater reduction in mortality in relation to pure diesel. This showed that the addition of 2G Ethanol promotes a reduction in toxicity considering the mixture of a commercial fuel with a renewable fuel of 1st and 2nd generation. However, the addition of HVO to pure diesel did not show favorable results, since there was a mortality of 100% of the organisms exposed to this sample, leaving a suggestion for future works.

[1] KOSLOWSKI, Luciano Andre Deitos et al. Assessment of the formation of polycyclic aromatic hydrocarbons and acute toxicity using diesel/butanol in a wet discharge pilot system for river boats. Journal of Environmental Chemical Engineering, v. 8, n. 2, p. 103532, 2020.

[2] DROTIKOVA, Tatiana et al. Polycyclic aromatic hydrocarbons (PAHs) and oxy-and nitro-PAHs in ambient air of the Arctic town Longyearbyen, Svalbard. Atmospheric Chemistry and Physics, v. 20, n. 16, p. 9997-10014, 2020.

[3] SANTHOSH, N. et al. Poultry fat biodiesel as a fuel substitute in diesel-ethanol blends for DI-CI engine: Experimental, modeling and optimization. Energy, p. 126826, 2023.

[4] JEONG, Seongho et al. Aerosol emissions from a marine diesel engine running on different fuels and effects of exhaust gas cleaning measures. Environmental Pollution, v. 316, p. 120526, 2023.9ARAUJO, G. S. et al. Toxicity of lead and mancozeb differs in two monophyletic Daphnia species. Ecotoxicology and environmental safety, v. 178, p. 230-238, 2019. Keywords: Fuels; Daphnia similis; toxicity.

Development of machine learning models to predict the uptake and transport of nanomaterials in plants

Dimitra-Danai Varsou[1, 2], Maria Antoniou[1], Panagiotis D. Kolokathis[1, 2], Georgia Melagraki[3], Iseult Lynch[2,4], and Antreas Afantitis[2,5]

1 NovaMechanics MIKE, Piraeus, Greece; 2 Entelos Institute, Larnaca, Cyprus; 3 Division of Physical Sciences and Applications, Hellenic Military Academy, Vari, Greece; 4 School of Geography, Earth and Environmental Sciences, University of Birmingham, Birmingham, UK; 5 NovaMechanics Ltd, Nicosia, Cyprus.
afantitis@novamechanics.com, i.lynch@bham.ac.uk

The existing concern regarding the possible risks from nanomaterials (NMs) to human health and environment impels the development of a solid NMs risk assessment framework. Computational approaches based on experimentally measured or theoretically calculated descriptors that encode NMs structural characteristics aim to provide a significant aid to prioritize NMs for experimental testing as part of a safe and sustainable by design (SSbD) strategy that optimises the materials properties based on the target application area. Recent efforts focus on the enrichment of existing nano-related datasets with computational descriptors that encode the knowledge of the NMs structure and composition and use of these novel-descriptors as additional input information in predictive modelling to gain deeper insights into the drivers of NMs behaviour and interactions in the environment. In the present work we introduce a novel nanoinformatics workflow using atomistic descriptors of NMs to build a machine learning scheme for the prediction of ecotoxicity-related endpoints in plants for NMs being developed for use in agriculture, such as the root concentration factor (RCF) which describes the amount of NMs taken up by plants from soil [1]. Atomistic descriptors are calculated using the NovaMechanics in-house software *NanoConstruct* (http://enaloscloud.novamechanics.com/riskgone/nanoconstruct/). In the proposed modelling workflow variable selection is used to refine the input parameters by removing those that overlap in terms of their predictive power and thus highlight those that are most important for interpreting how the selected nano-descriptors affect the log-transformed values of the RCF (endpoint). The proposed models (*k*NN, random forest regression models) are fully validated in accordance with the principles of the Organisation for Economic Cooperation and Development (OECD) for validation of predictive models and affords accurate predictions of the endpoint based on the different validation criteria used [2]. The entire modelling analysis was performed in Isalos Analytics Platform (https://isalos.novamechanics.com/) [3]. The use of atomistic NMs descriptors allows the fast screening of NMs as no additional experimental tests are needed to acquire these descriptors. We anticipate that the developed models will contribute to the safety-by-design of novel NMs for use in precision agriculture, and will be of use for stakeholders in Academia, Industry and Regulatory Agencies.

[1] X. Wang, L. Liu, W. Zhang, X Ma. Environ. Sci. Technol. 55, 11, 7491–7500 (2021).
[2] Golbraikh, A. and Tropsha, A. J. Mol. Graph. Model. 20, 269–276 (2002).
[3] Varsou, DD., Tsoumanis, A., Papadiamantis, A.G., Melagraki, G., Afantitis, A. Computational Methods in Engineering & the Sciences. (2023)

Acknowledgements: This work was supported by the EU Horizon 2020 programme via NanoSolveIT (grant agreement No. 814572) and RiskGONE (grant agreement No. 814425), with additional support from H2020 RISE project CompSafeNano (grant agreement No. 101008099). The authors would also like to thank the SPSAS NanoAgri&Enviro organising committee and corresponding funding parties for their support to the authors' participation in the advanced school.

Keywords: atomistic properties, machine learning, root concentration factor

The role of biogenic silica in soil microorganisms: A soil microcosm approach

Djanira R. Negrao[1,2], Carlos Driemeier[1], Charles W. Rice[2]
1Department of Agronomy, Kansas State University;
2Brazilian Biorenewables National Laboratory (LNBR/CNPEM), Brazil.

Many plant species accumulate silicon within their epidermal shoot tissues as micro-bodies of biogenic silica called phytoliths. Phytoliths have variable shapes and sizes (1 -300 µm), and their abundance depends on factors like plant species, soil type, and climate. Phytoliths represent one of the main sources of Si in soils if incorporated through litterfall or non-tillage management. However, there is a lack of knowledge of how biogenic silica-rich ashes influence the soil microbial community while soil aggregates are formed. This study uses a microcosm experiment to address this question using 3D-printed frames. Each frame was filled with 70 g silt clay loam soil with or without 1% wt. biogenic silica-rich ashes. The biogenic silica-rich ashes were prepared from the epidermis of the sugarcane internode and from the Miscanthus shoot. The sugarcane biomass was calcinated at 575ºC/4H, and the Miscanthus ash was 2x calcinated and acidic-digested between the calcination. The ashes and silt loam soil from conventional corn tillage were pre-sieved (<53 µm size). The six treatments consisted in using sugarcane or Miscanthus ash in separated experiments: 1) bulk soil, 2) soil, Blackwell switchgrass; 3) soil mixed with biogenic silica-rich ash; 4) soil, Blackwell switchgrass, and ash concentrated (3 cm φ diameter) at the soil surface; 5) soil mixed with biogenic silica-rich ash, Blackwell switchgrass; 6) soil mixed with biogenic silica-rich ash, Blackwell switchgrass, 3 µl mycorrhizal MycoApply® inoculum. The microbial community was accessed by analyzing the Neutral and Phospholipid Lipid Fatty Acid (NLFA/PLFA) obtained from the soil, and the root colonization of arbuscular mycorrhizae fungi (AMF). The phytolith-rich ashes mixed with soil positively affected Gram+ bacteria and AMF populations compared to all other treatments. Blackwell switchgrass shoot biomass was higher in the treatment with local biogenic silica-rich ashes (Tukey's test, $p < 0.05$). Using SEM imaging, all treatments had micro aggregates entangled by fungal hyphae, especially near the roots.

Keywords: Biogenic silica, phytoliths, soil aggregates, mycorrhizae, carbon sequestration

Combining sequential fractionation and spectroscopic techniques to unravel the contribution of plant species and soil microbes to phosphorus dynamics in the rhizosphere

Driss Touhami[1], Hudson. Carvalho[1] and Leonardus. Vergutz[1]
[1] *Chair of Soil Science, College of Sustainable Agriculture and Environmental Sciences, Mohammed VI Polytechnic University, Benguerir, Morocco.*
Driss.touhami@um6p.ma

Soil acidification and the exudation of organic anions and phosphatase enzymes are deemed to be the most important processes taking place in the rhizosphere of phosphorus (P) deficient plants. Roots-associated microorganisms replicate similar mechanisms to enhance P availability in the rhizosphere [1]. Previous studies have shown that there was no clear relationship between organic anion release and inorganic P acquisition and that plants and soil microbes can mobilize sparingly available and recalcitrant P fractions regardless of their chemical availability, as assessed by sequential P fractionation [2,3]. Current methods based on wet chemistry to assess soil P species are time-consuming, suffer from technical limitations, and do not reflect the true chemical speciation of P [4,5]. Therefore, more advanced techniques are required to better understand the influence of root and microbe processes in mobilizing different soil P species. In this regard, P-K edge XANES presents a useful tool to unravel changes in inorganic soil P fractions with minimal soil disturbance and high accuracy and precision. On the other hand, the use of ^{31}P NMR spectroscopy can provide detailed information on organic P species. Combining sequential fractionation and spectroscopic techniques can be effective in showing how plant species and soil microbes access different soil inorganic and organic P fractions at the soil-plant interface. This mechanistic understanding is important not only to improve P availability through management practices but also to enhance fertilizer P use efficiency through formulation technologies. In this study, two plant species (one grass and one legume) will be grown in two P-deficient soils with divergent inorganic and organic P content. The experiment will be carried out in rhizoboxes containing two compartments separated by a physical barrier. One side of the rhizobox will be filled with air-dried soil, while the other will be filled with the same soil gamma irradiated. After 30 days, the bulk and rhizosphere soil will be sampled and analyzed for soil pH, DOC, available P, exchangeable Ca, extractable Al and Fe, microbial biomass P, and acid and alkaline phosphatase enzyme activities. Roots with the remaining adhering soil will be immersed in a solution of $CaCl_2$ for organic anion determination. Soil P fractions will be assessed in both the bulk and rhizosphere soil by chemical fractionation, P-K edge XANES and ^{31}P NMR. Relationships between soil properties, organic anions, phosphatase enzyme activities, and different inorganic and organic P species will be determined using PCA analysis.

[1] Richardson AE, Lynch JP, Ryan PR, et al (2011) Plant and microbial strategies to improve the phosphorus efficiency of agriculture. Plant and Soil 349:121–156.
[2] Pearse SJ, Veneklaas EJ, Cawthray G, et al (2007) Carboxylate composition of root exudates does not relate consistently to a crop species' ability to use phosphorus from aluminium, iron or calcium phosphate sources. New Phytologist 173:181–190.
[3] Touhami D, McDowell RW, Condron LM (2020) Role of organic anions and phosphatase enzymes in phosphorus acquisition in the rhizospheres of legumes and grasses grown in a low phosphorus pasture soil. Plants 9:1185.
[4] Condron LM, Newman S (2011) Revisiting the fundamentals of phosphorus fractionation of sediments and soils. J Soils Sediments 11:830–840.
[5] Kar G, Hundal LS, Schoenau JJ, Peak D (2011) Direct chemical speciation of p in sequential chemical extraction residues using P K-edge X-ray absorption near-edge structure spectroscopy. Soil Science 176:589.

Keywords: Phosphorus cycling, rhizosphere, P-K edge XANES, 31P NMR.

National Public Policies for Nanotechnology and Advanced Materials: Critical Factors for Enhancing Effectiveness and Assertiveness

F. S. Bellucci[1]
[1] *Ministry of Science, Technology and Innovation of Brazil, Secretariat for Technological Development and Innovation, 70044-900, Brasília, Brazil.*
felipe.bellucci@mcti.gov.br

The promotion and development of science, technology, and innovation are constitutional premises stated in Article 218 of the Federal Constitution and in the framework of Law No. 10.973, dated December 2, 2004, known as the Innovation Law, and Decree No. 10.746, dated July 9, 2021, which established the Policy on Science, Technology, and Innovation for Advanced Materials. In this legal context, the fields of nanotechnology and advanced materials can be considered as two of the main enabling topics with significant potential for multi-sectoral innovation and economic development. However, formulating efficient and assertive public policies for complex topics remains challenging for developing countries. The objective of this study is to discuss the key elements that can positively or negatively impact the success of public policies in the areas of nanotechnology and advanced materials, considering various dimensions such as financial, economic, mobilizing, regulatory, security, social, and regional aspects. In the international context, literature review suggests that the most promising factors are: (i) creating favorable conditions for research institutes (RI) and companies interaction; (ii) education and training of human resources; (iii) encouraging international cooperation; (iv) fostering an entrepreneurial culture; (v) sustainable exploitation of biodiversity; (vi) promoting value addition to raw materials of mineral origin; (vii) arrangements among different levels of government; and (viii) promoting and public procurement in disruptive and strategic areas. After discussions and correlations with national challenges in the field of science, technology, innovation, and entrepreneurship, the most promising structural dimensions were: (i) promoting the creation of legal and sub-legal norms and governance structures for the development of nanotechnology and advanced materials; (ii) developing systems for processing, consolidating, intelligently disseminating information in these areas, given their diverse nature and stakeholders; (iii) education, training, mobility, and retention of specialized human resources; (iv) encouraging the establishment of new technology-based ventures in these fields; (v) fostering innovative environments and strengthening the relationship between RI and companies; (vi) enhancing collaboration, cooperation, and selected international alliances; (vii) utilization of digital technologies for accelerating, reduction of costs and improvement in nanotechnology and advanced materials; and (viii) promoting new disruptive areas within these fields. Thus, it is expected to provide support to the Ministry of Science, Technology, and Innovation of Brazil in formulating new public policies in the areas of nanotechnology and advanced materials [1,2], capable of creating conditions for the promotion of technology-based innovation, value addition, competitive advantage, and social and economic development in Brazil.

[1] Plano de Ação em CT&I para Tecnologias Convergentes e Habilitadoras - Vol. II - Materiais Avançados, Ministério da Ciência, Tecnologia e Inovação (2019).
[2] Plano de Ciência, Tecnologia e Inovação de Materiais Avançados, Ministério da Ciência, Tecnologia e Inovação (2022).
Acknowledgements: The author would like to thank the Ministry of Science, Technology, and Innovation of Brazil and the Brazilian Center for Research in Energy and Materials (CNPEM) for organizing the SPSAS NanoAgri&Enviro.

Keywords: Nanotechnology; Advanced Materials; Public Policies; and Enhancing Effectiveness.

Antimicrobial properties of chitosan-based microparticles against bacterial and fungal phytopathogens

F. A. Mesas[1], A. Torres Nicolini[2], M.C. Terrile[1], V.A. Alvarez[2], C.A. Casalongué[1], and J.R. Mendieta[1]

1 Universidad Nacional de Mar del Plata, Instituto de Investigaciones Biológicas, 7600, Mar del Plata, Argentina; 2 Universidad Nacional de Mar del Plata , Instituto de Investigaciones en Ciencia y Tecnologia de los Materiales, 7600, Mar del Plata, Argentina.

mesasflorencia@gmail.com

Traditional approaches to control phytopathogens have been based on toxic chemical compounds. The development of more sustainable and eco-friendly options is a great challenge in the present. In this sense, chitosan (CS)-based materials have emerged as a promising alternative for sustainable agriculture [1]. This study describes the synthesis and characterization, and includes a comparative biological analysis of antibacterial and antifungal activities from a set of CS microparticles (CS-MP). These particles were produced by ionic gelation using tripolyphosphate (TPP) as a crosslinker and during the synthesis process, different parameters were assayed (CS: TPP ratio, type, and time of agitation). CS-MPs were characterized by dynamic light scattering (DLS), Fourier transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and field emission scanning electron microscopy (FE-SEM). The obtained particles, designed as CS-MP1, CS-MP2, and CS-MP3 (0.19, 0.45, and 1.22 μm, respectively) exhibited contrasting zeta potential values (+7.57, +22, and +12.9 mV, respectively). We assayed the antimicrobial effect of these materials against two different phytopathogens, the bacterium model *Pseudomonas syringae* pv. *tomato* DC3000 (*P. syringae*) and the necrotrophic fungus *Fusarium solani* f. sp. *eumartii* (*F. eumartii*). Interestingly, a high value of zeta potential (CS-MP2) correlated with potent antimicrobial activity against these two types of phytopathogens, evidenced by lower IC_{50} and minimum inhibitory concentration (MIC) values. We discuss our findings in light of the material properties and opportunities to use CS-MPs as a new type of biomaterials in modern agriculture.

[1] F. N. Maluin and M. Z. Hussein, Molecules, 25(7), 1611 (2020).

Acknowledgements: This work was supported by UNMdP, ANPCyT, CIC, CONICET.
Keywords: chitosan, microparticles, antimicrobial activity.

Atmospheric microplastics and nanoplastics collected in cities in the state of São Paulo and their effects on lung cells

Gabriel M. Ferraz[1*], and Roberta C. Urban[1,2]
[1]Federal University of São Carlos, Department of Chemistry, Federal University of São Carlos, Brazil; [2]School of Geography, Earth and Environmental Sciences, University of Birmingham, United Kingdom
gabriel.ferraz@estudante.ufscar.br

The production and use of plastics have revolutionized the modern world, contributing for example to improvements in health through disposable medical equipment (PPE) [1]. Nonetheless, poor management of this waste results in already observed plastic pollution, including in the atmosphere. Although occupational diseases and the presence of these materials in human tissues have already been reported, the implications of atmospheric microplastics (MPs) and nanoplastics (NPs) on human health must be better understood [2-4]. This study aims to evaluate the presence of MPs in the atmosphere and their impacts on human health. Initially, the city of São Carlos, in the state of São Paulo, was selected for the samplings conducted in an elementary school in the center of the city. The MPs found were quantified and characterized physically and chemically, finding a concentration between 0 and 1.33 items m^{-3} for active sampling and 0 to 62.51 items m^{-2} day^{-1} for passive sampling. The main material was Polyester, followed by EVA. As a continuation of this study, the sample sites will be expanded to 3 cities, São Carlos, Indaiatuba, and Ribeirão Preto, all in the interior of the state of São Paulo and with different characteristics, with sites divided between remote regions and under the anthropic influence. In addition, a chromatographic method will be optimized and validated, using a Py-GC-MS, for the characterization and quantification of polymers, and also by μ-Raman. Furthermore, metabolites and corona proteins formed in lung cells exposed to MPs and NPs present in the atmosphere will be analyzed using in vitro cellular models of the air-liquid interface to simulate exposure by inhalation. Future results, mainly toxicological studies, are innovative and will help to evaluate the implications of MNPs in human health.

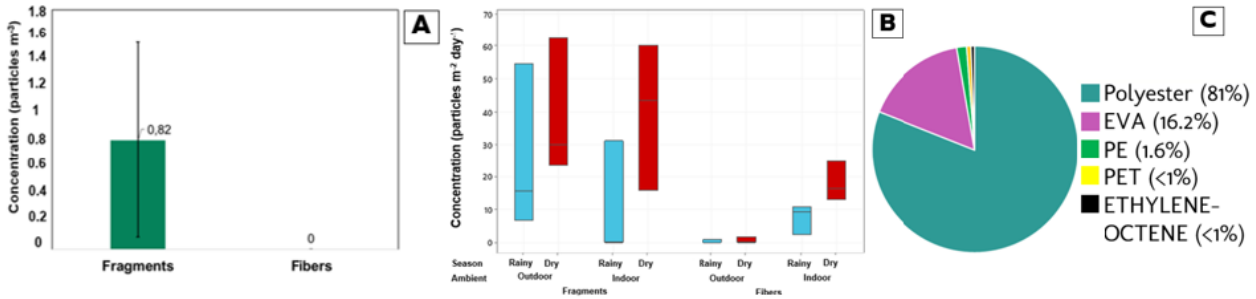

Figure A) MPs actively sampled concentration, B) MPs passively sampled concentration, and C) general composition of MPs collected

[1] J. C. Prata, J. P. da Costa, I. Lopes, A. C. Duarte and T. Rocha-Santos, Sci. Total Environ., 2020, 702, 134455.
[2] Y. Zhang, S. Kang, S. Allen, D. Allen, T. Gao and M. Sillanpää, Earth-Science Rev., 2020, 203, 103118.
[3] L. F. Amato-Lourenço, R. Carvalho-Oliveira, G. R. Júnior, L. dos Santos Galvão, R. A. Ando and T. Mauad, J. Hazard. Mater., 2021, 416, 126124.
[4] A. Kukkola, S. Krause, I. Lynch, G. H. Sambrook Smith and H. Nel, Environ. Int., 2021, 152, 106504

Acknowledgments: This work was supported by CAPES (Finance Code 001); FAPESP (#2018/04820-6, #2021/10187-7; #2022/03087-9); and INCTAA (CNPq #465768/2018-8; FAPESP, #2014/50951-4)

Keywords: Atmospheric microplastics, microplastic pollution, microplastic toxicity, air-liquid interface model

Prediction of the genotoxic potential of nanoparticles based on their descriptors

Ghada Tagorti[1] and Bülent Kaya[1]
[1] *Akdeniz University, Faculty of Sciences, Department of Biology, Antalya, Turkey.*
tagortig@gmail.com

Genetic toxicity includes a battery of assays to ensure the safety of chemicals for human health. Over the last decade, innovative approaches have been undertaken to reduce misleading positive results and to limit animal testing. Understanding the correlation between nanoparticle descriptors and the genotoxic potential of these chemicals is a promising alternative to new approach methodologies. Herein, a prediction of the genotoxicity was performed based on a reference dataset of five nanoparticles. The descriptors were based on the size distribution, hydrodynamic size, zeta potential, shape (1, rod; 2, sphere), and molecular weight of nanoparticles. Tested chemicals were classified as non-genotoxic (score=1) or genotoxic (score=2). Later, an unsupervised machine learning technique known as Principal Component Analysis (PCA) was conducted. This research demonstrates that some distinct descriptors could be associated with the genotoxic potential of nanoparticles. Overall, using computed prediction can contribute to more reliable and relevant results to improve the understanding of the risk assessment of nanoparticles.

Keywords: in silico, nanoparticle, PCA.

Synthetic nanoclays for use in water remediation: synthesis, characterization, and applications

Gipsy Peña Ramirez[1], L. Cano[1] and V. Álvarez[1]
[1] *Universidad Nacional de Mar del Plata (UNMdP), Instituto de Investigaciones en Ciencia y Tecnología de Materiales (INTEMA), 7600, Mar del Plata, Argentina.*
gipsy.pramirez@intema.gob.ar

Significant increase in nitrate levels in groundwater has been observed in many countries related to anthropic activities, as extensive agriculture, excessive application of nitrogenous fertilizers and inadequate wastewater treatment [1]. Nitrate is a potential human health hazard, especially to infants, causing the condition known as met-hemoglobinemia, also called blue baby syndrome [2]. Chronic accumulate of high level of nitrate and nitrite may also cause other health problems, for example some cancers and teratogenic effects [3]. Conventional treatments are not effective in eliminating these contaminants, the current alternatives for treatment are ionic exchange, reverse osmosis and electro-dialysis, however, these technologies are expensive, generate charged effluents and have a complex operation maintenance. For this reason, economic, effective and easy-to-use alternatives are required. Layered Double Hydroxides (LDH) are clay minerals that have properties such as high specific surface area, two-dimensional structure, ion exchange capacity, surface charge and high memory effect, [4] which allow HDL to be used as adsorbents for contaminants in water treatment. The synthesis of these nanoclays was carried out by coprecipitation, using three solutions (1.5M Mg/Al solution in a 3:1 ratio, another 1M Na_2CO_3 and 2M NaOH), subsequently the solid obtained was filtered, washed, dryed and calcined at 500°C. These solid was characterized by X-ray diffraction (XRD) and Fourier Transform Infrared Spectroscopy (FTIR). The XRD showed characteristic signals of hydrotalcite-type materials (Standard ref. 22-0700, JCPDS), showing for the synthesized LDH, fine and intense peaks for asymmetric flexions in the planes (003), (006) and (009), wide and with less intensity in the planes (015) and (018), and signals in planes (110) and (113). The XRD for the calcined LDH sample presents only two peaks corresponding to planes (200) and (220), evidencing the conversion of LDH into a mixture of oxides through calcination. For the LDH used, similar signals at fresh LDH were presented, with a slightly lower intensity, demonstrating the regeneration of the structure due to the adsorption of nitrates, after its calcination and use. The FTIR spectrum for the fresh LDH showed a wide absorption band between 3300-3700cm^{-1} due to the stretching of the OH groups present in the brucite-type sheets, another band at 1643cm^{-1} coming from the interlaminar water, a band at 1367cm^{-1} from the NO_3^- present in the interlaminar space and between 400-700cm^{-1} bands attributed to characteristic stretching and bending of hydroxyl groups attached to Al and Mg are observed. For calcined LDH, the signals corresponding to adsorbed water and nitrates are reduced, this is due to the collapse of the clay structure. For the LDH used, it is observed that the characteristic signals that were present in the fresh LDH are maintained, being the most intense band at 1367cm^{-1}, due to the adsorption of nitrates in the structure. The removal tests carried out on 100 ppm solutions and with an LDH dose of 100mg/50ml, showed removal percentages of nitrates between 94.58 and 99.23% and adsorption capacity (q) between 46.97 and 49.47mg/g, proving to be promising materials for nitrate removal.

[1] JW. Palko, DI. Oyarzun, B. Ha, M. Stadermann, JG. Santiago. Chem Eng J. 334, 1289-1296 (2018).
[2] S. Fossen Johnson. Nitrate Handbook, Environmental, Agricultural, and Health Effects. 347-355 (2022)
[3] A. De Sa, R. Lutchia, B. Srour, et al. Int J Epidemiol. 51, 1106-1119 (2022).
[4] D. Ivánová, P. Albert, J. Kavuličová. Appl Clay Sci. 152, 65-72 (2018).
Acknowledgements: The authors thank the funding sources provided by CONICET, ANPCyT and UNMdP and all non-teaching workers and technical support staff of our academic units and institutes.
Keywords: Layered double hydroxides, adsorption, nitrates, water.

Radiometric techniques as a tool to track pesticides delivered by nanoformulations in environment

Gustavo Vinícios Munhoz-Garcia[1], Vanessa Takeshita[1], Valdemar Luiz Tornisielo[1], Leonardo Fernandes Fraceto[2]

[1]*Center of Nuclear Energy in Agriculture, University of São Paulo, Piracicaba – São Paulo, Brazil.*
[2]*Institute of Science and Technology, São Paulo State University, Sorocaba – São Paulo, Brazil..*
gvmgarcia@usp.br

With the development of nanopesticides, the determination of environmental fate and toxicity is still a challenge because of the lack of protocols applied to the study of regulatory aspects of this technology. In this way, this work shows that protocols using carbon 14 (^{14}C) as a tracer, developed for conventional pesticides, can be useful in determining the environmental behavior and toxicity of nanopesticides. Some findings in the literature suggest that these techniques could be used to track pesticides delivered by nanosystems in processes such as absorption, translocation, sorption-desorption, leaching, and biodegradation. Radiometric techniques were first used by Takeshita et al. [1] and your research group to investigate the absorption and translocation of ^{14}C-atrazine-loaded with polycaprolactone in plants, confirming that absorption of nanoformulations was higher and faster than conventional formulations. The environmental behavior of metribuzin-loaded polymers and their availability in different soil systems were studied by Takeshita et al. [2, 3] using ^{14}C-metribuzin, showing the possibility of using radiolabeled pesticides to track active ingredients delivered by nanosystems in established soil systems. Such techniques can help to determine the environmental fate of nanopesticides by assessing both their behavior in the environment and their distribution among target and non-target organisms. Taken together, we highlight that radiometric techniques may be a powerful tool to be used in registration of pesticides delivered by nanosystems, ensuring a standard and safe evaluation of the impact of pesticide nanoformulations in agroecosystems before commercialization and application in agricultural areas.

[1] Takeshita, Vanessa, et al. "Foliar absorption and field herbicidal studies of atrazine-loaded polymeric nanoparticles."Journal of Hazardous Materials418 (2021): 126350.
[2] Takeshita, Vanessa, et al. "Development of a preemergent nanoherbicide: From efficiency evaluation to the assessment of environmental fate and risks to soil microorganisms." ACS Nanoscience Au 2.4 (2022): 307-323.
[3]Takeshita, Vanessa, et al. "Availability of Metribuzin-Loaded Polymeric Nanoparticles in Different Soil Systems: An Important Study on the Development of Safe Nanoherbicides." Plants 11.23 (2022): 3366.

Acknowledgements: This work was supported by São Paulo Research Foundation (FAPESP #2017/21004-5, #2019/04758-1, #2022/00509-0, #2022/0718-8).

Keywords: environmanetal fate, nanotechnology, analytical chemistry

Modification of Cd forms in volcanic soils by the effect of engineered nanoparticles (ENPs): An incubation study

Fuentealba, Isadora[1], A. Nicolás[1] and M. Karen[1]
1 Universidad de Santiago de Chile, Facultad de Química y Biologia, Laboratorio de Suelos y Medioambiente, Santiago, Chile.
Isadora.fuentealba@usach.cl

The presence of engineering nanoparticles (ENPs) in soil has aroused growing interest, where it has been estimated that the input of ENPs in soils worldwide is greater than 250,000 tons/m 3 [1]. When ENPs enter the soil, they can alter the vertical or horizontal transport of different analytes in the soil, ignoring the changes they can generate in the biogeochemical cycles [2]. For example, copper nanoparticles (CuNPs) used in agriculture as a fungicide agent, where their application ranges from 10 to 1000 mg/kg [2] and, depending on the soil pH, could dissolve Cu2+ , causing changes in the equilibrium that exist with other metals [2]. In the central-southern zone of Chile, 45% of the soils correspond to Ultisols, which have a pH ≤ 5.5 and mineralogy that favours the retention of P, so the application of phosphate fertilizers is a common practice to increase the amount of P. These fertilizers have a high proportion of Cd, which is incorporated into the soil. This work studied how CuNPs altered Cd fractionation in Ultisols at different incubation times. The soil was contaminated with Cd and incubated for 30 days. Then a dose of CuNPs was applied equivalent to 0.2% by mass concerning the soil 2.0 g of soils were taken 7, 30 and 60 days after the application of the ENPs, to study their fractionation [2]. The results indicated that the presence of CuNPs altered the distribution of Cd in the studied soils, observing that the availability of this metal increases with longer incubation times (60 days), where the fractions associated with weaker interactions increased 27 percentage points compared to the first seven days. In general, it was observed that at longer incubation times, Cd moves towards easily accessible surface groups in clays and organic matter, allowing its exchange with other ions in the soil. The information obtained is important to evaluate the impact of the residence time of CuNPs Ultisols. It can be used to develop regulations that aim to control this type of substrates better.

[1] Hochella, MF, Mogk, DW, Ranville, J., Allen, IC, Luther, GW, Marr, LC, McGrail, BP, Murayama, M., Qafoku, NP, Rosso, KM, Sahai, N., Schroeder, PA , Vikesland, P., Westerhoff, P., Yang, Y., 2019. Science. 80, 363.
[2] Gao, X., Spielman-Sun, E., Rodrigues, SM, Casman, EA, Lowry, GV, 2017. Environ. Sci. Technol. 51, 2226–2234.
Acknowledgements: The authors thank the support of PAI 77190014, FONDECYT 1190118

Keywords: Soil (Ultisol), Metallic Nanoparticles, Cd, Fractionation.

Development and characterization of nanocomposite film and its application in passion fruit

Jailton Ribeiro SANTOS JUNIOR[1]; Jailton Ribeiro SANTOS JUNIOR[1]; Luiz Carlos CORRÊA-FILHO[2]; Henriqueta Talita Guimarães BARBOZA[2]; Antônio Gomes SOARES[2]; Renata Valeriano TONON[2]; Lourdes Maria Corrêa CABRAL[2].

1 Federal Rural University of Rio De Janeiro – Rio De Janeiro; 2 Embrapa Food Agroindustry - Rio De Janeiro, Brazil
Email: juniorribeirodossantos@hotmail.com

The objective of this work was to develop and characterize chitosan films containing carnauba wax or rosin resin and zinc oxide nanoparticles, to be used as an active coating on passion fruit. The films were elaborated using the casting method. Chitosan solutions at 1.5% (w/v) were prepared in acetic acid at 1% (v/v) under mechanical agitation at 13,500 rpm. Carnauba wax or rosin resin 3% (w/v) solutions were prepared in 1% acetic acid and 1.5% (m/v) Tween 80 under magnetic stirring at 85°C at 1000 rpm and homogenized under mechanical stirring at 13,500 rpm. Mixtures were made with 800 ml of chitosan solution and 200 ml of carnauba wax or rosin resin under mechanical agitation at 13,500 rpm. Glycerol 0.36% (v/v) and ZnO_{nane} 0.05% (w/v) were added to the formulation. Six formulations were obtained, containing chitosan at 1.2% (w/v), glycerol at 0.36% (v/v), Tween 80 at 0.3% (v/v), varying the content of wax and resin at 0 or 0.6 (m/v) and ZnO_{nane} at 0 or 0.05 (m/v). The films were characterized according to their chemical and mechanical properties. All treatments resulted in homogeneous and flexible films. Films containing wax or resin were less transparent. The thickness of the films ranged from 86.00 ± 5.48 to 160.00 ± 13.09 µm. Films containing carnauba wax showed the lowest water content, 19.28% ± 0.04. The solubility values in water ranged from 12.36% ± 0.10 to 18.45% ± 0.57%. The films containing carnauba wax and wax plus ZnO_{nane} were the least soluble, presenting values of 12.36% ± 0.10 and 14.59% ± 0.55 respectively. Regarding the degree of sorption, films containing resin plus ZnO_{nane}showed the highest degree of sorption 45.59% ± 0.95 when compared to the other treatments that ranged from 29.18% ± 1.15 to 41.77% ± 2, 83. Given the above and taking into account the solubility aspects, films containing carnauba wax and wax with ZnO_{nane} can be used as a coating on passion fruit.

Acknowledgements: This work was supported by FAPERJ and CAPES.
Keywords: post-harvest, nanotechnology, shelf life.

Development of transparent thin films of semiconductor oxides for surface functionalization

J.G. Cuadra[1], S. Molina-Prados[2], Gladys Mínguez-Vega[2], Ana. C. Estrada[3], T. Trindade[3], C. Oliveira[4], M.P. Seabra[5], J. Labrincha[5], S. Porcar[1], R. Cadena[1], D. Fraga[1], J.B. Carda[1]

1 Department of Inorganic and Organic Chemistry, Universitat Jaume I, Avda. Sos Baynat s/n, 12071, Castellon, Spain
2 GROC-UJI, Institute of New Imaging Technologies, Universitat Jaume I, Avda.Sos Baynat s/n, 12071 Castellon,Spain
3Department of Chemistry, CICECO-Aveiro Institute of Materials, University of Aveiro, 3810-193 Aveiro, Portugal
4 Department of Biology, CESAM, University of Aveiro, Campus Universitário de Santiago,3810-193, Aveiro, Portugal
5 Materials and Ceramic Engineering Department, CICECO, University of Aveiro, Campus Universi-tário de Santiago, 3810-193 Aveiro, Portugal
Corresponding author: jcuadra@uji.es

In recent years, there has been a significant increase in the interest surrounding thin film technology due to its broad range of applications, such as in photovoltaic solar cells [1], energy storage [2], heterogeneous photocatalysis, and antimicrobial action [3]. Additionally, the COVID-19 pandemic has made the development of antivirus and antimicrobial materials a critical priority worldwide. Consequently, the ability to functionalize various surfaces without altering their optical properties has become a primary concern. To address this need, transparent TiO2 thin films coated with Ag NPs were synthesized using two industrially applicable techniques, pulsed laser ablation (PLAL) and spray pyrolysis, without the use of high vacuum. These thin films were deposited on glass to create materials with photocatalytic and antimicrobial properties while maintaining high transparency. To analyze the structural, morphological, and optical properties of the thin films, Grazing incidence X-ray diffraction (GIXRD), Raman spectroscopy, Scanning electron microscopy (SEM), and ultraviolet-visible spectroscopy were used. The presence of NPs on the TiO2 surface was identified using Transmission electron microscopy (TEM). The thin films exhibited a transmittance value of over 80%. Next, the photocatalytic capacity of the synthesized thin films was evaluated by measuring the degradation of Rhodamine B (RhB) under UV light irradiation. The presence of Ag NPs on the TiO2 surface resulted in an improvement in photocatalytic properties, with a 99% degradation of RhB achieved in just 210 minutes under UV light. Furthermore, these transparent thin films demonstrated high antimicrobial activity on Gram-negative bacteria when irradiated with UV light for 4 hours, effectively killing 93% of these bacteria.

Keywords: Transparent thin films; Spray pyrolysis; Laser ablation; Antimicrobial activity; Photocatalysis.

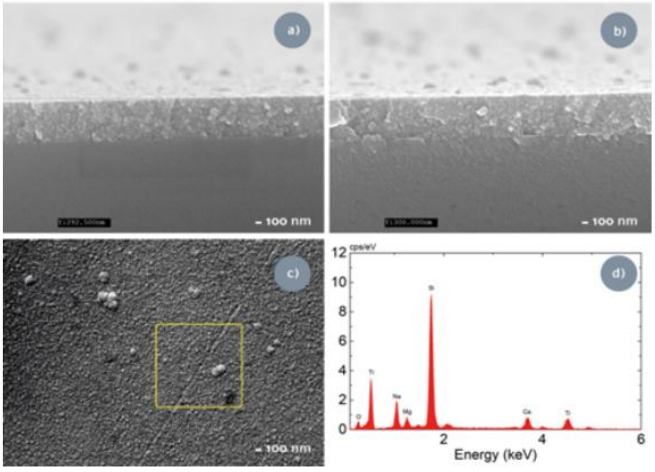

Figure 1: SEM images for the cross section of (a) TiO2 transparent thin films, (b) TiO2-Ag NPs, (c) top surface of TiO2, and (d) EDS spectra for the surface of TiO2.

Acknowledgements: The authors would like to acknowledge the financial support provided by the Spanish Ministry of Economy and Competitiveness via the Ministry of Science and Innovation's "R&D&I Projects" in the State Programs

for Knowledge Generation and Scientific and Technological Enhancement of the R&D&I System and R&D&I Aimed at Society's Challenges under the Spanish National Plan for Scientific and Technical Research and Innovation (2019-2020). The funding source for the project PID2020-116719RB-C43 was MCIN/EAI/10.13039/501100011033. The author of this article would also like to thank Projects TED2021-130963B-C22 financed by AEI/10.13039/501100011033/ European Union NextGenerationEU/PRTR and FOTO-CER project funded by CDTI, supported by the Ministry of Science and Innovation and funded by the European Union - NextGenerationEU - through the measures included in the Recovery, Transformation and Resilience Plan.The authors would also like to acknowledge the Universitat Jaume I's "Serveis Centrals d'Instrumentació Cientfica" (SCIC) for their assistance in characterising the materials. This work was conducted as part of the CICECO-Aveiro Institute of Materials project, UIDB/50011/2020, UIDP/50011/2020, and LA/P/0006/2020, which was supported by national funds via FCT/MCTES (PIDDAC). Ana C. Estrada would like to acknowledge the FCT-funded research contract costs, which were covered by National funds (OE) via FCT, I.P., as part of the framework contract outlined in Article 23, points 4, 5, and 6 of Decree-Law 57/2016, dated 29 August, as amended by Law 57/2017.
Keywords: Transparent thin films; Spray pyrolysis; Antimicrobial activity; Photocatalysis

Development of an eco-friendly pesticide containing microbial extracts to combat insect pests

Janaína Brandão Seibert[1,2] , Italo Delalibera Jr. [2] , Ana Paula Ruani[1] , Lulliana Thalita Franco[1] , João Batista Fernandes[1] and Moacir Rossi Forim[1]

1 Universidade Federal de São Carlos, Departamento de Química, 13565-905, São Carlos, Brazil. 2Universidade de São Paulo – ESALQ, Departamento de entomologia, 13418-900, Piracicaba, Brazil

jana_seibert@hotmail.com

Leaf-cutting ants are highlighted as agricultural pests due to their practice of collecting plant material for nest maintenance, which generates great economic losses [1]. In order to get around this situation, conventional agriculture is characterized by the excessive application of synthetic insecticides, which generally cause environmental pollution, health problems in humans and animals and can give rise to resistant microorganisms [2]. Faced with this problem, researchers have given great attention to the discovery of alternatives to these harmful synthetic compounds, and natural products are a promising source of new pesticides [3]. The present work aimed to evaluate the potential of extracts of microorganisms in combating leaf-cutting ants. For this purpose, yeasts of the genus Phialophora were cultivated in axenic cultures and in co-cultures with the fungus Escovopsis microspora. The LC-MS/MS analyzes of the extracts allowed the annotation of 11 substances for the mono and co-culture of P. attae and 8 substances for P. capiguarae. The fungicidal effect was evaluated using the agar diffusion assay and only the extracts obtained from P. attae showed an inhibitory effect on Leucoagaricus gongylophorus. The insecticidal action on atine ants was stipulated by the acetylcholinesterase inhibition test and the toxicity of the extracts was evaluated both on human cells and on eucalyptus seeds. A lower IC50 value for the enzymatic assay was found for the co-culture of E. microspora and P. attae, as well as, this extract proved to be more selective due to lower toxicity rates. Despite the possibility of using microorganism extracts to combat leaf-cutting ants, natural products have some physicochemical limitations related to their low stability and solubility in water [4]. To enable the use of these extracts, nanoemulsion systems were developed based on the phase inversion emulsification method. The formulations showed particle size between 86 and 95 nm, polydispersity index lower than 0.2 and negative zeta potential. Furthermore, all nanoemulsions were stable after submitting the accelerated stability test. Therefore, the data reinforce the viability of developing products containing extracts of microorganisms that can be used as an alternative in the fight against leaf-cutting ants.

[1] T. M. C. Della Lucia, L. C. Gandra and R. N C. Guedes, Managing leaf-cutting ants: peculiarities, trends and challenges, Pest Manag. Sci. 70, 14-23 (2014).
[2] J. Montoya-Lerma, C. Giraldo-Echeverri, I. Armbrecht, A. Farji-Brener and Z. Calle, Leaf-cutting ants revisited: towards rational management and control, Int. J. Pest Manag. 58, 225–247 (2012).
[3] A. Hussain, M. Rizwan-Ul-Haq, H. Al-Ayedh and A. M. Al-Jabr, Mycoinsecticides: potential and future perspective, Recent Pat. Food, Nutr. Agric. 6, 45-53 (2014).
[4] R. Watkins, L. Wu, C. Zhang, R. M. Davis and B. Xu, Natural product-based nanomedicine: recent advances and issues. Int. J. Nanomedicine 10, 6055-6074 (2015).

Acknowledgements: This work was supported by Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq process 150578/2021-0) and Fundação de Amparo à Pesquisa do Estado de São Paulo (FAPESP process 2020/00819-3 and 2022/04694-6)
Keywords: nanotechnology, pesticide, leaf-cutting ants, microorganism extract

Synthesis and Characterization of Two-Dimensional Nanostructures of Ilmenite: Exploring Magnetism and Optical Properties for Nanotechnology Applications

Jéssica V. Alves[1], Antonio M. L. M. Costa[2] and Natasha M. Suguihiro[1]
1 Universidade Federal do Rio de Janeiro - Campus UFRJ-Duque de Caxias Prof. Geraldo Cidade, RJ, Brazil;
2 Universidade Federal do Rio de Janeiro, LIPCat, RJ, Brazil.
jessica.vicenti@ufrj.br

Two-dimensional nanomaterials are materials composed of a single layer of atoms or a few atomic layers. They hold great promise for applications in nanotechnology due to their size- and morphology-dependent physical properties. Ilmenite ($FeTiO_3$), which is an abundant mineral on Earth, demonstrates paramagnetic behavior at room temperature. However, recent research reports indicate that 2D nanostructures of ilmenite, in the form of nanosheets, exhibit weak magnetism caused by surface spin anisotropy. Consequently, these structures are being investigated as a model for nanomagnetism in two dimensions [1]. Moreover, these nanosheets can also display alterations in their optical properties, such as an increased bandgap [3], making them promising for environmental remediation applications through photocatalytic processes. In this study, ground ilmenite was utilized as a precursor in alkaline hydrothermal synthesis, employing NaOH as an alkaline agent. Several parameters were controlled, including time, temperature, and mass of the precursor. The resulting synthesis products were characterized using X-ray diffraction, as well as scanning and transmission electron microscopy. The results revealed the complete conversion of ground ilmenite into 2D nanostructures. Photocatalytic tests were conducted to assess the degradation of methylene blue using both UVB and UVA light sources with an intensity of 9W. The tests demonstrated a superior photocatalytic performance compared to the ground material. The
magnetic and optical properties of the synthesized nanostructures are currently being evaluated to establish correlations with their microstructure.

[1] A Non-van der Waals Two-Dimensional Material from Natural Titanium Mineral Ore Ilmenite. Aravind, P.B., et al. Chemistry of Materials, 2018, 30, 17, 5923-5931.
[2] Structural, electronic and elastic properties of FeBO3 (B = Ti, Sn, Si, Zr) ilmenite: a density functional theory study. Ribeiro, R. A. P., et al. The Royal Society of Chemistry, 2014, RSC Adv. 4, 104, 59839-59846.
[3] Semiconductor quantum dots: Technological progress and future challenges. F. Pelayo García de Arquer, et al. Science 373, eaaz8541 2021.

Acknowledgements: This work was supported by Fundação de Amparo à Pesquisa do Estado do Rio de Janeiro (FAPERJ).

Keywords: Two-dimensional nanomaterials, ilmenite, photocatalytic processes.

Co-exposure studies of iron oxide nanoparticles and glyphosate in *Poecilia reticulata* fish support safe environmental remediation strategies

J. M. de Lima-Faria[1], V. C. da Silva[1], D. S. T. Martinez[2], S.M.T de Sabóia-Morais[1]
[1] Laboratory of Cellular Behavior (LCC), Institute of Biological Sciences (ICB), Federal University of Goiás (UFG), 74690-900, Goiânia, Brazil; [2] Brazilian Nanotechnology National Laboratory (LNNano), Brazilian Center for Research in Energy and Materials (CNPEM), 13083-100, Campinas, Brazil.
joaolima@discente.ufg.br

Iron oxide nanoparticles (IONPs) are promising nanomaterials for the remediation of glyphosate (GLY) and Glyphosate-based Herbicides (GBH) contaminated aquatic environments, since IONPs can adsorb GLY on the surface, therefore it is necessary to know the toxicity and recovery capacity of aquatic organisms undergoing IONP and GLY co-exposure. In this sense, this work presents a collection results of bioaccumulation results and biological responses in fish *Poecilia reticulata* under exposure to IONPs and co-exposure to IONPs+GLY and IONPs+GBH, as well as presents the physiological behavior of the animals in post-exposure periods with only reconstituted water [1-2]. Characterization of IONPs resulted in crystalline shaped nanoparticles with an average individual size of 2.90±0.84 nm, hydrodynamic size in ultrapure water of 66.60±0.17 r.nm, and zeta potential of -55.40±7.40 mV [1]. The experimental design had 60 females in 60-liter tanks organized into the groups: Control with reconstituted water; $FeCl_3$ at 0.3 mgFe/L (IFe); IONPs at 0.3 mgFe/L; IONPs+GBH1 with 0.3 mgFe/L of IONPs and 0.65 mgGLY/L of GBH; IONPs+GBH2 with 0.3 mgFe/L of IONPs and 1.30 mgGLY/L of GBH and; IONP+GLY with 0.3 mgFe/L of IONPs and 0.65 mg/L of GLY. The experimental duration was 42 total days, 21 days exposure and 21 days post exposure with collections every 7 days. The multiple biomarker analysis included: histological evaluations; calculation of the histopathological index of the liver; analysis of cell ultrastructure and lipid distirubution in hepatocytes by SEM and TEM and; study of iron accumulation in the fish body by ICP-OES. The results showed that the inflammatory responses are more persistent in all treatments, but are accentuated in the animals treated with IFe, IONP+GBH1 and IONP+GBH2 but despite this the total histopathological index showed a tendency to decrease during the post-exposure period [1]. Added to these results are the decrease in lipids in hepatocytes and the decrease in iron concentration in the animals' bodies at the end of postexposure [2]. It is possible to conclude that treatments at the concentrations used cause reversible damage to the liver tissue of *P. reticulata*, so that the accumulation of iron in the body of the individuals decreases in the post-exposure and accompanies the recovery of the animals, therefore, this set of data supports the safe use of maghemite IONPs in environmental remediation strategies - since there is a tendency for the animals to recover in 21 post-exposure days - and opens the way for studies with longer exposure and post-exposure time intervals to confirm the trend of full recovery of the animals.

[1] Lima-Faria, J. M. de, Silva, V. C. da, Chen, L. C., Martinez, D. S. T. & Sabóia-Morais, S. M. T. de. Co-exposure of iron oxide nanoparticles with glyphosate herbicides in Poecilia reticulata: Fish liver damages is reversible during iron accumulation and elimination period. Chemosphere 328, (2023).
[2] Faria, J. M. de L., Guimarães, L. N., Silva, V. C. da, Lima, E. C. de O. & Sabóia-Morais, S. M. T. de. Recovery trend to co-exposure of iron oxide nanoparticles (γ-Fe2O3) and glyphosate in liver tissue of the fish Poecilia reticulata. Chemosphere 282, (2021)

Acknowledgements: Work supported by Fundação de Amparo a Pesquisa do Estado de Goiás and Coordenação de Aperfeiçoamento de Pessoal de Níviel Superior. Authors would like to thanks LabMic-UFG, CRTI-UFG, LabCOMNUFG

Keywords: co-exposure, postexposure, environmental remediation, iron oxide nanoparticles.

Non-targeted characterization of soil organic matter using electrospray ionization - Fourier transform - ion cyclotron resonance - mass spectrometry

João Vitor dos Santos[1], Aleksandar I. Goranov[1], Lais G. Fregolente[2], Marcia C. Bisinoti[3], Ladislau Martin-Neto[4], Patrick G. Hatcher[1]

1 Old Dominion University, Department of Chemistry and Biochemistry, Norfolk, United States of America; 2 Brazilian Centre for Research in Energy and Materials, Brazilian Nanotechnology National Laboratory, Campinas, Brazil; 3 São Paulo State University, Department of Chemistry, São Jose do Rio Preto, Brazil; 4 Embrapa Instrumentation, National Laboratory of Agri-Photonics, São Carlos, Brazil.

j1dossan@odu.edu

One of the most recent advances in materials science has been the development of nanomaterials, which have now been applied in various environmental fields, including agriculture. Nano-agrochemicals, including various fertilizers, pesticides, and fungicides, are now being used and are under investigation of how they interact with naturally present molecules within the soil organic matter (SOM) [1]. It has been demonstrated that nano-agrochemical particles acquire a coating on their surfaces from their first interaction with SOM, which largely occurs due to nano-eco interactions [2]. Novel methods are required to study these interactions to fully understand the fate of nano-agrochemicals in the environment. One of these is electrospray ionization - Fourier transform - ion cyclotron resonance - mass spectrometry (ESI-FT-ICR-MS), a high-resolution MS technique for the molecular characterization of soil organic matter (SOM) and its different fractions, such as humic acids (HA) and dissolved organic matter (DOM). This method is widely used in environmental science and soil science for the analysis of complex organic matter in natural systems [3]. Here, we have evaluated the molecular features of HA from Amazonian anthropogenic soils (ADE) and DOM from pasturelands in Brazil using ESI-FT-ICR-MS. The molecular differences between the two SOM pools are remarkable. Pasture DOM is composed primarily of lignin-like compounds, followed by lipid-like and carbohydrate-like compounds. In contrast, ADE HA are composed primarily of condensed aromatic-like compounds, followed by lignin-like compounds. DOM and HA are comprised primarily of CHO-type molecules, followed by CHON and CHOS. However, molecular formulas of HA appear to be more complex than DOM. These molecular results establish a baseline for future studies that assess the interactions between DOM or HA with nano-agrochemicals.

[1] J. Zhao, M. Lin, Z. Wang, X. Cao, and B. Xing. Engineered nanomaterials in the environment: Are they safe?, Critical Reviews in Environmental Science and Technology, 51:14, 1443-1478, 2021.
[2] L. Xu, M. Xu, R. Wang, Y. Yin, I. Lynch, and S. Liu. The Crucial Role of Environmental Coronas in Determining the Biological Effects of Engineered Nanomaterials. Small, 16, 36, 1–23, 2020.
[3] R. L. Sleighter and P. G. Hatcher. The application of electrospray ionization coupled to ultrahigh resolution mass spectrometry for the molecular characterization of natural organic matter. Journal of Mass Spectrometry, 42, 559-574, 2007.

Acknowledgements: The authors are grateful for the financial support provided by the São Paulo Research Foundation (FAPESP, grant numbers: 20/04938-7 and 21/08362-5) and the Frank Batten Endowment fund to Dr. Patrick G. Hatcher by Old Dominion University (Norfolk, VA).

Keywords: Dissolved Organic Matter, ESI-FT-ICR-MS, Molecular Characterization

Phosphorus foliar fertilisation in P-deficient maize – significance of leaf surface properties for P-uptake

Jon Niklas Henningsen[1], Victoria Fernández[2] and Karl Hermann Mühling[1]
1 Institute of Plant Nutrition and Soil Science, Kiel University, Hermann-Rodewald-Straße 2, 24118 Kiel, Germany
2 Systems and Natural Resources Department, School of Forest Engineering, Universidad Politécnica de Madrid, 28040 Madrid, Spain
jnhenningsen@plantnutrition.uni-kiel.de

The essential plant nutrient phosphorus (P) is key for numerous structures and processes in crops and its deficiency can severely restrict yield and quality. As soil P availability for plant uptake is often limited, foliar P application can be an alternative means of supplying P to the plants during the growth period, but foliar uptake mechanisms are poorly understood. Maize (*Zea mays* L.) is one of the most important crops worldwide, being the staple food for hundreds of millions of people. However, maize is also particularly susceptible to P deficiency in early stages of development. Therefore, the aim of this PhD project was to investigate the possibilities of foliar P application as a complement to soil fertilisation in P-deficient maize, with a particular focus on the significance of leaf surface properties for foliar P uptake. Three subprojects were developed in which the following was investigated (1) the basic efficiency of a P foliar application in P-deficient maize plants (2) the main leaf surface properties influencing P uptake and (3) the influence of leaf surface properties in combination with foliar fertiliser properties on P foliar uptake. For this purpose, leaf surfaces and structures were characterised using various methods (SEM, TEM, CA, FTIR) and the subsequent P absorption was evaluated depending on the respective surface properties (ICP-MS/OES). Furthermore, the influence of P uptake via the leaf on physiological processes was determined (LICOR LI-6400XT/LI-600). Foliar P application significantly increased photosynthetic rate and enhanced biomass production. Also, elemental analysis revealed increased tissue P concentrations compared to P-deficient plants. However, the positive effect on photosynthetic rate and P concentration was only temporary and vanished a few days after foliar treatment, in addition, the level of P-sufficient plants could not be reached, hence the plant functionality of P-deficient plants could not be restored. In order to determine the reasons for the limited efficiency of P foliar application, the leaf surface was then characterised. It was revealed that although P deficiency has no influence on the properties of the leaf surface, the cultivar does. Variety P7948 did not develop epicuticular wax crystals from the 4th leaf onwards and was thus wettable. Variety DKC3096, however, was only wettable from the 6th leaf. Wettability was the decisive factor for P foliar uptake.
While in P7948 the P concentration level of P-sufficient plants was achieved after P foliar treatment, this was not the case for DKC3096. On the unwettable leaves of DKC3096, also the P form was a deciding factor. In general, for unwettable leaves, P uptake was increased by the addition of a surfactant, whereby a solution containing a surfactant and a P salt with low deliquescence relative humidity (DRH, K_2HPO_4) resulted in the highest P uptake compared to a salt with high DRH (KH_2PO_4). In summary, the efficacy of a P foliar application is strongly dependent on the leaf and P fertiliser properties, with wettability and form of the P salt being of key importance.

Acknowledgements: J.N. Henningsen receives a grant from Konrad-Adenauer Foundation, which is gratefully acknowledged.

Keywords: P foliar fertilisation, leaf surface properties, maize

Biopesticides nanoformulations for the control of pathogens and pests

Jonathan Dias de Lima[1], D. Fernandez[2] and M.O. Rodrigues[1]
1 Universidade de Brasília - UnB, Laboratório de Inorgânica e Materiais - LIMA, Instituto de Química - IQ, Brasília, DF 70.910-900, Brazil; 2 IRD - Institut de Recherche pour le Développement, PHIM Plant Health Institute, Univ Montpellier, IRD, CIRAD, INRAE, Institut Agro, Montpellier, France.
dias12lima@gmail.com

Agriculture is one of humanity's oldest activities, with the current challenge of developing sustainable agriculture combined with agricultural overproduction. Plant pests and diseases are causing significant losses in Brazil's cotton, soybean, coffee, tomato, and corn production. Nanotechnology brings to agriculture the development of nanobiopesticides that aims to serve as a pest treatment agent and soon increase productivity. Thus, this project aimed to develop nanoformulations based on Carbon dots (C-dots): C-dots@OEC, C-dots@OECr, C-dots@OELD, and C-dots@Cu. C-dots, copper nitrate, essential oils (OEs) of citronella (OEC), clove (OECr), and sweet orange (OELD) were used in the preparation of nanobiopesticide formulations. These formulations were characterized by fluorescence spectroscopy, infrared, and transmission electron microscopy techniques, and the essential oils used in the preparations had their chemical compositions determined by GC/MS. The nanoparticles employed in these formulations were morphologically spherical C-dots with a size of 5.3 nm. The prepared nanoformulations have similar characteristics, as shown by fluorescence and infrared spectroscopy graphs. According to the characterization of the EOs, it was possible to identify that the main bioactive compounds are β-citronellal, β-citronellol, geraniol, eugenol, β-caryophyllene, and limonene. In the fungicidal activity, all the nanoformulations inhibited the germination of urediniospores of *Hemileia vastatrix* (coffee leaf rust) ($p < 0.05$). In the nematicidal evaluation, there was a higher mortality rate of J2 larvae of root-knot nematodes (*Meloidogyne incognita*) when the C-dots@OECr nanoformulation was used (84%). In conclusion, the developed nanoformulations demonstrated a biopesticide character for agricultural pests. This project resulted in the production of a patent filed in 2020 entitled "*BIOPESTICIDE NANOFORMULATIONS BASED ON SECONDARY METABOLITES AND MICRONUTRIENTS, RELATED PRODUCTION METHOD AND RELATED USE TO CONTROL PATHOGENS AND PESTS*" under application number **BR102020002179A2**.

Acknowledgements: This research was supported by Embrapa Recursos Genéticos e Biotecnologia, Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (Capes) and Institut de Recherche pour le Développement (IRD).

Keywords: C-dots, nanoparticles, coffee leaf rust, root-knot nematode.

Effect of surface chemistry on the adsorption of dyes in carbon nanotube. A supramolecular perspective

José Arévalo-Fester[1,2] and Alexander Briceño[1]

1Instituto Zuliano de Investigaciones Tecnológicas (INZIT). Km 15, La Cañada de Urdaneta, Estado Zulia, Venezuela.
2Instituto Venezolano de Investigaciones Científicas (IVIC), Centro de Química. Laboratorio de Síntesis y Caracterización de Nuevos Materiales. Apartado 21817, Caracas 1020-A, Venezuela.
Email:joseduardo27@gmail.com

Controlled hydrophilic carbon-based sorbents from functionalized carbon nanotubes (MWCNT-COOH) were developed via hydrothermal glucose-coated carbonization, mixing MWCNT with glucose in different weight ratio. Methyl violet (**MV**), methylene blue (**MB**), alizarin yellow (**AY**) and methyl orange (**MO**) were used as dye models for adsorption studies. Comparative dye adsorption capacity onto the pristine (MWCNT-raw) and functionalized (MWCNT-COOH-11) CNTs was evaluated in aqueous solution. These results revealed that MWCNT-raw are capable of adsorbing either anionic or cationic dyes. In contrast, an induced selective cation dye adsorption capacity is significantly enhanced on multivalent hydrophilic MWCNT-COOH, in comparison to pristine surface. This ability can be tuned to the selective adsorption of cations over anionic dyes or between anionic mixtures from binary systems. An insight into adsorbate-adsorbent interactions, shown that hierarchical supramolecular interactions dominate the adsorption processes, which is ascribed to chemical modification from switching hydrophobic to hydrophilic surface, dye charge, temperature and potential matching multivalent acceptor/donor capacity between chemical groups in the adsorbent interface. The dye adsorption isotherm and thermodynamics on both surfaces were also studied. Changes in the Gibbs free energy ($\Delta G°$), enthalpy ($\Delta H°$) and entropy ($\Delta S°$) were evaluated. Thermodynamic parameters and endothermic on MWCNT-raw, whereas the adsorption process on MWCNT-COOH-11 revealed that adsorption processes were spontaneous and exothermic, accompanied with a significant reduction of entropy values as consequence of multivalent effect. This approach provides an eco-friendly, low-cost alternative for the preparation of supramolecular nanoadsorbents with unprecedented properties to achieve remarkable selective adsorption independent of the presence of intrinsic porosity [1,2].

[1] Lehn, J. M. Supramolecular Chemistry: Concepts and Perspectives; VCH: Weinheim, Germany, 1995; pp 1−206.
[2] José Arévalo-Fester and Alexander Briceño. ACS Omega 2023, 8, 12, 11233–11250.

Acknowledgements: The authors thank FONACIT for financial support through Project PEI-2013002269. Also, they thank T. González, Y. Díaz and E. Cañizales (Intevep-PDVSA) for technical assistance.

Keywords: Carbon nanotubes, Supramolecular Chemistry, Dyes Adsorption

Nanoparticle Arrays Generated Using Mesoporous Films as Templates

Josefina Morrone[1], M. C. Fuertes[2] and A. Zelcer[2,3]
1CIBION, CONICET, Ciudad de Buenos Aires, Argentina
2Gerencia Química & INN, Centro Atómico Constituyentes, Comisión Nacional de Energía Atómica, CONICET, San Martín, Buenos Aires, Argentina
3ECyT, Universidad Nacional de San Martín, San Martín, Buenos Aires, Argentina
josefinamorrone@gmail.com

By the emergence of robust methods to synthesize materials with controlled nanometric porosity, the so-called nanocasting or hard-templating was developed, which uses porous materials as molds to generate various nanostructures[1,2]. This method of preparation has the advantage that the size of the nanoparticles (NPs) is limited by that of the nanopores, and that they are trapped within the porous system, resulting in a mechanically robust and chemically stable composite material. These nanocomposites are of interest for application in sensing and catalysis[3,4,5]. Mesoporous thin films were synthesized by deposition of silicon dioxide with controlled porosity and pore sizes. These films were deposited by spin coating, using the sol-gel process combined with the self-assembly of surfactants[6]. Iron NPs supported into mesoporous thin film were synthetized following a two-step method using a volatile precursor. First, the mesoporous film and the iron precursor were placed into a chambre but not in direct contact. This chamber was submitted to high vacuum and the heated at 130°C. Finally, the nanocomposite was removed from the chamber and treated at 200°C to decompose the precursor into the oxide. Its subsequent decomposition allowed the localized formation of NPs in a scalable and controlled manner. The filling of the pores was studied by X-ray reflectometry to determine the change in the electronic density of the material, as well as the variation in the accessible porosity. UV-visible and FT-IR spectra were recorded in order to determine the presence of colored species and changes in the chemical structure, respectively.

[1] Lu, A.-H. and F. Schüth, Nanocasting: A Versatile Strategy for Creating Nanostructured Porous Materials. Advanced Materials, 2006. 18(14): p. 1793-1805.
[2] Deng, X., K. Chen, and H. Tüysüz, Protocol for the Nanocasting Method: Preparation of Ordered Mesoporous Metal Oxides. Chemistry of Materials, 2017. 29(1): p. 40-52.
[3] Violi, I.L., et al., Gold nanoparticles supported in zirconia-ceria mesoporous thin films: A highly active reusable heterogeneous nanocatalyst. ACS Applied Materials & Interfaces, 2015. 7(2): p. 1114-1121.
[4] Coneo Rodríguez, R., M.M. Bruno, and P.C. Angelomé, Au nanoparticles embedded in mesoporous ZrO2 films: Multifunctional materials for electrochemical detection. Sensors and Actuators B: Chemical, 2018. 254: p. 603-612.
[5] Coneo Rodríguez, R., et al., Copper nanoparticles synthesis in hybrid mesoporous thin films: Controlling oxidation state and catalytic performance through pore chemistry. Applied Surface Science, 2019. 471: p. 862-868.
[6] Brinker, C.J., et al., Evaporation-Induced Self-Assembly: Nanostructures Made Easy. Advanced Materials, 1999. 11(7): p. 579-585.

Acknowledgements: This work was supported by Agencia I+D+i (PICT 2017-1133, PICT 2019-01615). The authors would like to thank G. Zbihlei for the TEM images.

Keywords: Metallıc Nanopartıcles, Mesoporous Thın Fılm, Nanopartıcle Array

Elaboration of a multilayer film of Agar/Chitosan/Metal nanoparticles and nanoemulsion of garlic extract as promising food packaging.

Josué Delgado[1], Gema González[1], Antonella Macias[1], Lola de Lima[1] and Javier Alvarez[1]
[1] *Yachay Tech University, School of Physical Sciences and Nanotechnology, 100119, Urcuqui, Ecuador*
josue.delgado@yachaytech.edu.ec

Antimicrobial packaging is a type of packaging that contains antimicrobial agents that kill or inhibit the growth of bacteria, fungi, and other microorganisms. The aim of antimicrobial packaging is to increase the shelf life of food products and prevent food waste. The use of antimicrobial packaging can be particularly beneficial for perishable foods such as meats, dairy products, and fresh fruits and vegetables[1]. In this study, multi-layer films of agar/chitosan-garlic nanoemulsion/agar with metal nanoparticles were fabricated as antimicrobial packaging. The idea of using a multilayer system is to have a sustained release of garlic active compounds which has demonstrated antibacterial, antifungal and antioxidant properties[2]. Moreover, the combination of agar and chitosan results in a polymeric complex due to the opposite electrical charges of these materials, which leads to the formation of a polyelectrolyte complex with unique properties. The multilayer arrangement were fabricated layer by layer using a casting method and the nanoemulsion was prepared by mixing garlic extract and citric acid and then reducing the emulsion size by physical mechanisms using ultrasound. The multilayer system is illustrated in Fig 1. The films were then characterized using FTIR and the antimicrobial properties were tested using the Kirby Bauer method. Different nanoparticles were tested for antimicrobial activity: CeO2, Ag, ZnO. The nanoparticles with the best performance were incorporated in the agar films and then composite materials were tested to study the synergic effect of garlic extract and nanoparticles. The antimicrobial activity of nanoparticles was Ag>ZnO>CeO2. On the other hand, garlic extract showed good antifungal activity on Candida. Therefore, the combination of garlic extract with nanoparticles is a potential material for food antimicrobial packaging protection.

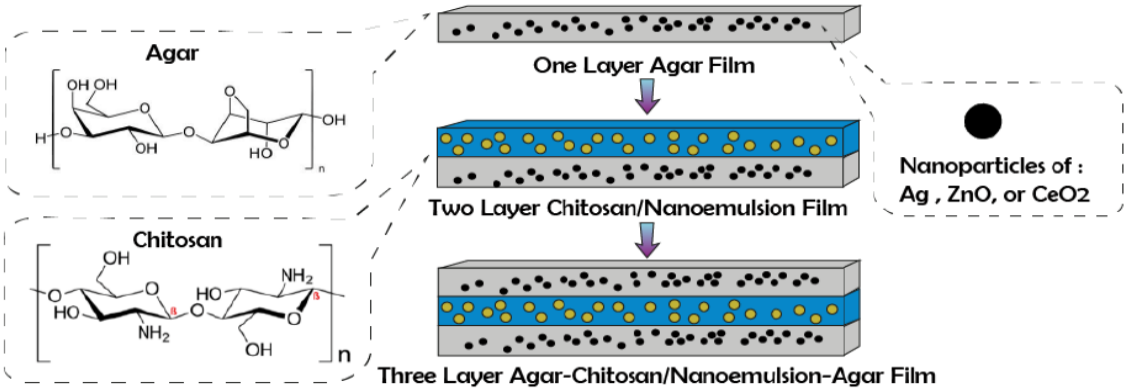

Figure 1. Schematic representation of the multilayer system.

[1] Zhang, X., Ismail, B. B., Cheng, H., Jin, T. Z., Qian, M., Arabi, S. A., ... & Guo, M. (2021). Emerging chitosan-essential oil films and coatings for food preservation-A review of advances and applications. Carbohydrate Polymers, 273, 118616.
[2] Hasssanzadeh, H., Alizadeh, M., & Rezazad Bari, M. (2018). Formulation of garlic oil-in-water nanoemulsion: antimicrobial and physicochemical aspects. IET nanobiotechnology, 12(5), 647-652.

Acknowledgements: The authors would like to thank Yachay Tech University for the use of its laboratories.
Keywords: Chitosan, Garlic, Antimicrobial, Films.

Synthesis and characterization of chitosan nanoparticles functionalized with rose bengal for photosensitized degradation of a model pollutant

Julieta L. Sacchetto[1], Cristian. M.O. Lépori[2], R. Dario Falcone[1] and Walter A. Massad[1]
[1] Instituto para el Desarrollo Agroindustrial y de la Salud (IDAS), Dpto. de Química, Facultad de Ciencias Exactas, Físico-Químicas y Naturales, Universidad Nacional de Rio Cuarto, 5800, Rio Cuarto Argentina. [2] Dpto. de Química, Facultad de Ciencias Exactas, Físico-Químicas y Naturales, Universidad Nacional de Rio Cuarto, 5800, Rio Cuarto Argentina.
jsacchetto@exa.unrc.edu.ar

Phenolic pollutants are compounds of demonstrated environmental importance as aquatic pollutants, these are generally colorless, therefore the degradation by photosensitized processes become relevant. One of the main drawbacks of photosensitization processes in a homogeneous medium is the extraction of the dye once the reaction has been completed. For this reason, the development of polymeric dyes that can be easily removed from the reaction media is a very interesting alternative for photosensitized processes in environmental applications. Rose Bengal (RB) is a dye that in water generates singlet oxygen with a quantum yield of 0.75, while chitosan (CS) is a natural and biodegradable organic polymer easily functionalized. The main goal in the present work is the immobilization of the sensitizer RB in CS nanoparticles that we will call nRBCS. Thus,1-Ethyl-3-(3-dimethylaminopropyl) carbodiimide (EDC) was used for the synthesis of RBCS composite. EDC was employed for the formation of amide bonds, which is formed between the RB carboxyl group and the CS amino group. Once RBCS was synthesized, the polymer dye was crosslinked with sodium tripolyphosphate under controlled stirring conditions to obtain nRBCS. Free sensitizer nanoparticles was obtained for comparison. An important feature is that nRBCS is stable at pH 7 and is readily removed by centrifugation. A benzenetriol, 1,2,3 trihydroxybenzene (THB) were selected to test the photosensitized activity of the synthesized nanoparticles. THB are known to be reactive to singlet oxygen ($^1O_2$) in homogeneous media. Nanoparticles was characterized by UV-Vis absorption spectroscopy, fluorescence and NMR technique. By NMR technique both the synthetic route and the nanoparticle size were established. Particularly, using DOSY technique, the diffusion coefficient of the nanoparticles was determined and applying the Stokes-Einstein equation, the size of the CS (320 nm) and nRBCS (357 nm) nanoparticles were obtained. UV-Vis spectroscopy was used to evaluate the oxidation of THB by photosensitized of nRBCS. The degradation of THB was observed in the presence of the free sensitizer as well as when the synthesized nanoparticles were used. Sodium azide scavenger was employed to assess the presence of $^1O_2$ contribution in the degradation process. In addition, laser flash photolysis studies revealed that nanoparticles electronically excited states are involved in the generation of $^1O_2$. Preliminary results exposed that nRBCS exhibit a higher quantum yield of fluorescence and a lower triplet exited state quantum yield than free RB. The use of the nRBCS in photosensitized process represents a great advantage over free dye. The nRBCS has a higher stability at pH 7 allows it to be used for longer periods. It does not present the diffusion problems intrinsic to heterogeneous media. The photosensitized degradation of THB revealed that the synthesized nanoparticles may generate $^1O_2$ and degrades the benzenetriol. Finally, one of the most promising characteristics of these nanoparticles, is that it can be extracted after photosensitized reaction, leaving the aquatic environments free of pollutants or pigments and provides a practical solution for those who are immersed in the subject of environment remediation.

Acknowledgements: This work was supported by CONICET, FONCYT and UNRC.

Keywords: photosensitized processes, nanoparticles, photodegradation

Thermal treatment to increase the solubility of ultrapotassic syenite for use as a potassium fertilizer

Khawla Aıt Harrouch[1], Abdellatif Elghal[1], Leonardus Vergutz[2]
[1] *Mohammed VI Polytechnic University, Geology, and Sustainable Mining Institute, Ben Guerir, Morocco*
[2] *Mohammed VI Polytechnic University, Chair of Soil Science, Ben Guerir, Morocco*
Khawla.Aıtharrouch@um6p.ma

Along with nitrogen and phosphorus, potassium is essential for plant growth. It plays a critical role in many physiological processes, including photosynthesis, protein synthesis, and water regulation. Water-soluble potassium sources are geographically concentrated in a few numbers of nations. Thus, many potash fertilizer's importing countries are reliant on potash fertilizer supplies. Exploring non-conventional resources such as K-bearing silicates can be one of promoting initiatives to meet future potash demand. However, the locked structure of alumina-silicate minerals and the very low leaching rate of macronutrients compared to conventional salts present a real challenge. Extensive studies have been undertaken on potassium extraction using the roasting route, as the most effective route for K release there was too much focus on manufacturing and application of silicate fertilizers, whereas limited knowledge of material science had been obtained, about the deep investigation in mineralogical changes and the mechanism during the thermal treatment. Our work aims to enhance the solubility of potassium-rich igneous rock using the thermal process with a better knowledge of the reaction's mechanism. Our project will recover potassium, through chlorination roasting followed by water leaching. Chloride melting agents such as $CaCl_2$ will be used for this purpose. The effects of various experimental parameters such as temperature, time, mass ratio, and particle size distribution, on the potassium extraction process, will be evaluated using a statistical design of experiments. The characterizations of roasted, leach liquor, and leach residue samples will be carried out using a series of analytical and spectral techniques such as X-ray diffraction, X-ray Absorption Near Edge Structure, and scanning electron microscopy equipped with energy-dispersive X-ray spectrometer to evaluate the mineral phase changes and chemical alteration after the thermal process. Further studies for optimization will be carried out using response surface methodology to optimize the factors for maximizing potash recovery. The end-product will estimate the effectiveness of the calcination process to produce highly soluble K mineral from a low solubility mineral and confirm the potential of those silicate minerals for K fertilizer production, with further evaluation of the plant availability of the K in soils.

Keywords: K-bearing Silicate minerals, Chlorination Roasting, potash recovery, K fertilizers.

X-ray Absorption Spectroscopy in Optical Materials: From Trivial Data Analysis to Machine Learning

L. U. Khan[1], Z. U. Khan[2,3], H. F. Brito[3] and S. J. A. Figueroa[4]

[1] *Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan.*

[2] *Department of Biochemistry, Institute of Chemistry, University of São Paulo (USP), Zip Code 05508-000, São Paulo-SP, Brazil.*

[3] *Department of Fundamental Chemistry, Institute of Chemistry, University of São Paulo (USP), Zip Code 05508-000, São Paulo-SP, Brazil.*

[4] *Brazilian Synchrotron Light Laboratory (LNLS), Brazilian Center for Research in Energy and Materials (CNPEM), 13083-970, Campinas-SP, Brazil.*

latifullah.khan@sesame.org.jo

The quantum confined semiconductor nanocrystals and luminescent rare earths materials are important photoemitters in visible to near-infrared spectral region, manifesting wide photonic applications in light-emitting diodes (LEDs), telecommunications, optical lasers, display devices, optical quantum memories, photovoltaic cells, night vision devices and medical diagnostics. In order to get detailed insight into the photo-physical characteristics of these materials, it is very important to probe the local atomic/electronic structure of the metal's sites. X-ray absorption spectroscopy (XAS) can be very potent to probe the metal ions, from oxidation state/electronic structure in near edge region (XANES) to the local atomic structure order around the photoabsorber in extended region (EXAFS). A crucial relation between the X-ray photon and optical photon is manifested by X-ray excited optical luminescence (XEOL), demonstrating the fundamental mechanism of the conversion of X-ray energy absorbed by the system to optical photons. XEOL is often used together with XANES to provide site specificity and reveal the electronic structure and optical properties of the wide range of luminescent materials. In present work, we present a new strategy based on modern data science PyFitIt machine learning package to quantitatively gain insight on the three-dimensional local structure of the luminescent materials from XANES simulation [1], in correlation with classical Continuous Cauchy wavelet transform (CCWT), conventional EXAFS fit analyses [2] and optical properties.

[1] L.U. Khan, Z.U. Khan, L. Blois, L. Tabassam, H.F. Brito and S.J.A A. Figueroa, Inorganic Chemistry, 62, 2738–2750 (2023).
[2] Z.U. Khan, M.K. Uchiyama, L.U. Khan, K. Araki, H. Goto, M.C.F.C. Felinto, A.O. De Souza, H.F. Brito, M. Gidlund and P.D. Mascio, ACS Applied Nanomaterials (ACS), 6, 3767–3780 (2023).

Acknowledgements: The authors acknowledge the financial support by Royal Society of Chemistry Inclusion and Diversity Fund (RSC). Sirius the Brazilian Synchrotron Light Laboratory (LNLS), part of the Brazilian Center for Research in Energy and Materials (CNPEM) and BM-08 XAFS/XRF Beamline of SESAME Synchrotron Light Source for XAFS data measurements.

Keywords: X-ray absorption fine structure, Machine learning, Optical spectroscopy

Implementing FAIR and CARE Data Principles in Life Cycle Assessment: supporting the UN Sustainable Development Goals

L. Cristiana Gheorghe[1], Jonathan D. Oldfield[1] and Iseult Lynch[1]
1 School of Geography, Earth and Environmental Sciences, University of Birmingham, Edgbaston, B15 2TT Birmingham, UK .
l.c.gheorghe@bham.ac.uk

Introduction: Life Cycle Assessment (LCA) is the most powerful tool for evaluating the environmental impact of materials, products, processes, activities or services over their entire life cycle. LCA is thus a critical tool underpinning progress towards the United Nations' Sustainable Development Goals (UN SDGs). Although efforts are underway to improve the accuracy of LCAs, there are currently many limitations, with lack of data for the LCA inventory of inputs and outputs, which leads to poor quality LCA results, being the most significant. The FAIR data principles are key to increasing data accessibility and re-usability. In the context of the SDGs, with their focus on developing economies, inclusion of indigenous knowledge is essential, as incorporated in the CARE principles. Life Cycle Assessment: A Systematic Assessment Tool Life cycle inventory (LCI) is the comprehensive accounting of the inputs and outputs, such as rawmaterial production, manufacture, distribution, use and disposal including all intervening transportation steps necessary or caused by the product's existence. The inputs and outputs are referred to as Elementary flow and concern mainly raw materials, energy, land or water use, while the outputs track the released emissions to air, water, and soil, as well as solid waste generation. FAIR and CARE Principles for data

Figure 1: Overview of the FAIR and Care Principles briefly (GIDA - Global Indigenous Data Alliance)[1]

FAIR (Findable, Accessible, Interoperable and Reusable) is a set of guiding principles that enable and increase the reuse of data by humans and machines. Some of the principles apply to the technical solutions for indexing and sharing data, while some concern the standards and norms of the specific research communities (Schultes, 2022). The 'CARE Principles for Indigenous Data Governance' (Collective Benefit, Authority to Control, Responsibility, and Ethics) reflect the crucial role of data in advancing innovation, governance and self-determination among Indigenous Peoples (Carroll et al., 2020). By following the FAIR and CARE principles, data sets suitable for use in LCA can be developed, allowing researchers to perform more accurate LCA and stakeholders to make informed decisions about the environmental impacts of products and services. Conclusions: Applying the FAIR Data principles systematically when generating LCA inventories and data of relevance for LCA will increase the amount of data available for conducting an LCA. In addition, FAIR sharing of data can lead to more efficient re-use of research data, including in targeting the SDGs where FAIR and Open data is essential for sustained progress. Sharing data will advance the LCA field and its applications. To embrace life cycling thinking and the circular economy and to contribute to the SDGs let's start by making our data FAIR, enabling re-use of existing data for completer and more reliable LCA results.

[1] GIDA - Global Indigenous Data Alliance (https://www.gida-global.org/care)
Acknowledgements: This work has received funding from the European Union's Horizon 2020 research and innovation programme via NanoSolveIT Project under grant agreement No 814572 and CompSafeNano Grant agreement No: 101008099Keywords: Life Cycle Assessment, FAIR and CARE Data, Sustainable Development Goals

Foliar application of different iron sources on cucumber seedlings (*Cucumis sativus* L.): investigation of absorption, transport, and chlorophyll recovery

Laura Galvan Nuevo[1], Eduardo Ferreira Molina[2], and Hudson Wallace Pereira de Cravalho[1]
1 Universidade de São Paulo, Laboratório de Instrumentação Nuclear, Centro de Energia Nuclear na Agricultura, 13416-000, Piracicaba, Brazil; 2 Universidade de Franca, Departamento de Química, 14404-600, Franca, Brazil.
lauranuevo@usp.br

Recent studies show that the use of nanomaterials in agriculture has a promising scenario, in which these particles can bring greater nutrient use efficiency compared to traditional sources, being used in seed coating, through the soil or trough foliar application. In addition, further studies need to be conducted in order to understand the advantages of these materials [1]. In this sense, this work aim to evaluate the efficiency of foliar applied Fe nano-polymers in comparison with Fe sulfate and Fe chelate in the process of absorption, transport, and chlorophyll recovery, through X ray fluorescence spectroscopy techniques (XRF and μXRF), in addition to visual observations and quantum efficiency of photosystem II analysis. The element iron was chosen to indicate the possible better absorption caused by the nano-polymer, since studies report an improvement in vegetative growth parameters due to increased chlorophyll content after foliar applications of different sources of Fe in plants with deficiency of this micronutrient [2,3]. Cucumber plant leaves (*Cucumis sativus* L.) will be treated with Fe sulfate, Fe ethylenediamine tetra-acetic acid (EDTA), and Fe nano-polymers developed at Universidade de Franca, all treatments have iron concentration of 500 mg. L-1. The nano-polymers were synthesized in two formulations: encapsulated Fe sulfate and encapsulated Fe EDTA, with the aim of promoting a slow release of this nutrient on the leaf surface. Due to this characteristic of nano-polymeric formulations, the expected results of this work are higher Fe absorption rate, consequently, higher chlorophyll recovery and higher transport rate, allowing this nano-polymer to be used in formulations with other nutrients, aiming at greater efficiency of foliar applications in crops.

[1] H. W. P. Carvalho, et al. Are nanomaterials leading to more efficient agriculture? Outputs from 2009 to 2022 research metadata analysis. Environ. Sci.: Nano, 9, 3711-3724 (2022).
[2] F. Yunta, I. Martin, J. J. Lucena and A. Gárate. Iron chelates supplied foliarly improve the iron translocation rate in Tempranillo grapevine. Communications in Soil Science and Plant Analysis, 44:1-4, 794-804 (2013).
[3] A. W. M. Mahmoud, et al. Foliar application of different iron sources improves morpho-physiological traits and nutritional quality of broad bean grown in dandy soil. Plants, 11, 2599 (2022).

Acknowledgements: This work was supported by the Foundation for Agrarian Studies “Luiz de Queiroz” (FEALQ) and by The São Paulo Research Foundation (FAPESP).

Keywords: Nanomaterials; Foliar fertilizers; XRF.

Cytotoxic and genotoxic effects of zinc oxide nanoparticles on *Allium cepa* roots: an analysis of particle size dependence

Leandro Oliveira Araujo[1], Thalíta Hellen Nunes Lima[1], Valter Aragão Do Nascimento[2], Samuel Leite De Oliveira[1], Anderson Rodrigues Lima Caires[1]

1 Grupo de Óptica e Fotônica, Instituto de Física, Universidade Federal de Mato Grosso do Sul, 790070-900 Campo Grande, MS, Brazi; 2 Laboratory of Spectroscopy and Bioinformatics Applied to Biodiversity and Health, Faculty of Medicine, Federal University of Mato Grosso do Sul, Campo Grande, Mato Grosso do Sul 79070-900, Brazil.
leandro.araujo@ufms.br

Nanotechnology is a growing field in technological, scientific, and biological areas. In particular, zinc oxide nanoparticles (ZnONPs) have received great attention because of their unique properties and their application in numerous commercial products [1]. The production, use, and disposal of ZnONPs are attracting great concern due to their inevitable release into the environment, generating several uncertainties about their fate, behavior, and toxicity. As plants are at the base of the ecosystem, it is necessary to study the toxic effects of ZnONPs on plants [2]. In this context, the present study aimed to evaluate the environmental toxicity of ZnONPs by using meristematic cells of Allium cepa seeds as a plant model; ZnONPs (< 50 and <100 nm) were characterized by Transmission Electron Microscopy (TEM), in which we determined their shape, and mean diameter. The data demonstrated that the nanoparticles presented toxic effects on Allium cepa cells, showing that the smaller nanoparticles were more cytotoxic and genotoxic than the large ones. The results also suggest that the mechanisms of toxicity are related to the production of reactive oxygen species (ROS) and the release of ions. This statement is confirmed by the preliminary results of ROS production by ZnONPs in the presence of Dihydroethidine (DHE), a ROS production marker, as well as by the Zn^{2+} ions release determined by the dialysis experiments.

[1] Mueller, N.C., Nowack, B., 2008. Exposure modeling of engineered nanoparticles in the environment. Environ. https://doi.org/10.1021/ es7029637.
[2] Rossi, L., Fedenia, L.N., Sharifan, H., Ma, X., Lombardini, L., 2019. Effects of foliar application of zinc sulfate and zinc nanoparticles in coffee (Coffea arabica L.). https://doi.org/10.1016/j.plaphy.2018.12. 005

Acknowledgements: This research was funded by, CNPq and, SISFÓTON-MCTI, FUNDECT and for financial support.– Brazil, CAPES.

Keywords: Nanoparticles, Zinc Oxide, Allium cepa

Surface Functionalization of Thin-Film Composite Membranes with Photoactive Lignin-Derived Carbon Dots for Improved Antimicrobial Properties

Liu Yang, Andreia F. Faria*
Engineering School of Sustainable Infrastructure & Environment, Department of Environmental Engineering Sciences, University of Florida, P.O. Box 116580, Gainesville, FL, 32611-6580, USA
**Corresponding Author (E-mail: andreia.faria@essie.ufl.edu, Tel: 352-392-7104)*

Fresh water is an essential resource for human well-being and the natural environment, but due to industrial development and climate change there is growing concern regarding potable water scarcity and quality. In light of this, there is an urgent need for economical and efficient technologies for producing potable and supplementing current water supplies. Reverse osmosis (RO) membrane filtration will be crucial for addressing these concerns as it can be used to both desalinate water (supplement water supplies with brackish/saline water) and capture contaminants of emerging concern (such as microplastics, pharmaceuticals/personal care products, etc.) Thin-film composite (TFC) membranes are the gold standard for commercial RO filtration, but they are vulnerable to biological contamination. Bacteria present in the feed water can attach to the membrane surface, reproduce, and develop into a biofilm which is difficult to remove and significantly reduces membrane performance. After a mature biofilm has formed, membranes must be replaced which drives up the cost of applying membrane technology. For this reason, addressing biofouling is critical for increasing the efficiency of RO systems. To improve membrane lifespan and performance, we proposed modifying TFC membranes lignin-based nanomaterials. Lignin is hydrophilic, naturally derived, and can even be extracted from waste streams to form useful materials-carbon dots (CD). In this study, lignin was obtained through sequential hydrothermal processes from elephant grass biomass. We demonstrate a simple and environmentally friendly route to synthesize fluorescent CD by the hydrothermal treatment of lignin with the assistance of H2O2. Then, we use polydopamine (PDA) self-polymerization reaction to bond photoactive antibacterial CD and TFC membrane to achieve synergism between photovoltaic bactericidal and biocide against biofouling. The functionalized membranes are extensively characterized by spectroscopy and microscopy techniques to confirm the successful combination of CD, and assessed its effect on the membrane's intrinsic transport properties. The bound CD impart strong antibacterial activity to TFC membranes, as evidenced by plate counting using Escherichia coli (Gram-negative) and Bacillus subtilis (Gram-positive) as model bacteria in contact with the membrane surface. Our results highlight the potential use of CD as multifunctional antimicrobial agents to increase biofouling resistance in TFC membranes while enhancing the desalination capacity of TFC membranes for a variety of environmental applications.

Keywords: Water quality, thin-film composite membrane, sustainable nanomaterials, membrane modification

Controlled recovery of biomolecules from model and complex biotechnological systems using magnetic nanoparticles

Lucía Abarca Cabrera[1], Sonja Berensmeier[1] and Paula Fraga-García[1]
[1] *Technical University of Munich, Bioseparation Engineering Group, School of Engineering and Design, Garching bei München, Germany.*
l.abarca@tum.de

Magnetic nanoparticles (MNP) have the ability to adsorb different types of molecules, including proteins, lipids, and polysaccharides. Therefore, they are a useful bioseparation tool; however, selective adsorption of a target molecule or group of molecules onto MNPs is still a challenge. Efforts have been made to obtain this specificity by performing surface functionalization, which is common in chromatography materials. Nonetheless, functionalization increases the price, rendering nanoparticles less suitable for certain large-scale applications. Our final goal is to trigger selectivity for specific biological components in complex environments using inexpensive bare inorganic nanomaterials. In this work, we offer a broad picture of adsorption of biomolecules onto MNPs (1) starting with a defined model system and then (2) moving onto very complex systems such as biotechnological broths, in which the microorganism dictates the biomolecule composition. Firstly, we quantify the whole content adsorbed through individual analytical methods and perform surface characterization and secondly, we identify particular molecules that show selective interaction by SDS-PAGE and mass spectrometry, in order to understand if their intrinsic characteristics, such as their pI, hydrophobicity or size, drive the adsorption. The model mixture comprises BSA, sodium oleate and dextran as model molecules representing proteins, lipids and carbohydrates, respectively. We have determined that pH plays a key role for adsorption: in the case of proteins, mainly due to electrostatic interactions; for the fatty acids due to the formation of structures; and in the case of the sugars, such as dextran, no influence of pH was observed. We used microalgal lysates, i.e., Microchloropsis salina as very complex systems and the results reveal that proteins, lipids and carbohydrates spontaneously bind onto the MNP surface. We obtained selectivity by using additives such as cysteine and sodium oleate, changing the partition of solute molecules between the liquid and the surface of the solid phase. Here, we present hints regarding the interactions between different types of molecules and bare inorganic nanomaterials, offering a perspective to predict the formation of the biocorona. This work aims to stimulate the creation of a new generation of smart nanomaterials that are selective in highly complex environments, and at the same time, that could switch their selectivity depending on the medium properties and the processing steps, in order to separate the whole biomass through the fractionation of valuable products and to design sustainable downstream processes.

[1] Abarca-Cabrera, L., Fraga-García, P. & Berensmeier, S. Biomater Res. 25, 12 (2021).
[2] Abarca-Cabrera, L., Xu, L., Berensmeier, S., Fraga-García, P. ACS Appl. Bio Mater. 6 (2023).

Acknowledgements: The authors would like to thank CONACYT for financially supporting the project.

Keywords: controlled recovery, biomolecules, nanoparticles

Probabilistic material flow analysis of nano-TiO_2 releases in Mexico

Luis Mauricio Ortiz-Galveza[2,*], Alejandro Caballero-Guzman[3], Carla Lopes[1], Ernesto Alfaro-Moreno[1]

1 NanoSafety Group, International Iberian Nanotechnology Laboratory, 4715-330 Braga, Portugal
2 Plentzia Marine Station University of the Basque Country, Areatza Pasealekua 48620 Plentzia –Bizkaia Basque Country, Spain
3 Green Sustainability Strategic Consulting, Mexico-Switzerland, 8180 Bülach, Switzerland
** Current address: Empa, Technology & Society Laboratory, 9014 St. Gallen, Switzerland*
ernesto.alfaro@inl.int

Nowadays, many companies globally commercialize Engineered Nanomaterials (ENMs) or products containing ENMs, known as nano-enabled products. At the same time, the concern about the potential risks and negative impacts related to the release of ENMs into the environment is under investigation. For this reason, researchers have developed methodologies to estimate mass concentrations of ENMs released in different regions of the world, such as in Europe and the US. However, ENMs or nano-enabled products are also produced or imported in developing countries, such as in Mexico. Therefore, in the present study, a Probabilistic Material Flow Analysis (PMFA) model was developed as a first attempt to estimate the mass flows of nanosized titanium dioxide (nano-TiO_2) released in Mexico, for the year 2015. The model describes mass flows of released nano-TiO_2 during the life cycle of sunscreens, coatings, ceramic, and other nano-enabled products, including the flows through the solid waste and wastewater management systems, and the transfer of nano-TiO_2 to three environmental compartments (air, soil, and surface water). Using probability distributions, the PMFA incorporates the uncertainty related to the input data. According to the model, the largest flows occur to the surface water, landfill, and soil (Fig. 1), targeted as the main "hot-spots", where living organisms might be exposed to nano-TiO_2. The model needs further improvements due to some data gaps in certain stages of the life cycle, for instance, the solid waste management and the reused wastewater manipulation for irrigation purposes. Finally, the PMFA elaborated in this study can be modified to assess other ENMs releases and can be useful for further investigation in fate modelling and environmental risk assessment.

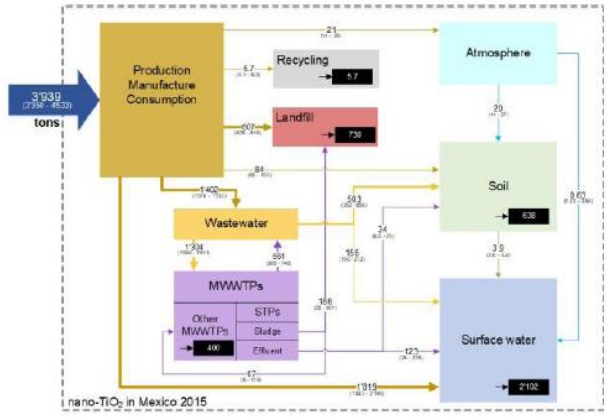

Figure 1. Mass flow representation of nano-TiO_2 in Mexico, 2015. Flows are described in tons/y, as arrows, with the means of probability, in which the thickness illustrates their magnitude; numbers in parenthesis are the 15th and 85th percentiles; and, black boxes indicate sink compartments. MWWTPs stands for Municipal Wastewater Treatment Plants and STPs for Sludge Treatment Plants.

Acknowledgements: This research was funded by the European Union's H2020 project Sinfonia (N.857253). SbDToolBox, with reference NORTE-01-0145-FEDER-000047, supported by Norte Portugal Regional Operational Programme (NORTE 2020), under the PORTUGAL 2020 Partnership Agreement, through the European Regional Development Fund. Luis Mauricio Ortiz-Galvez would like to thank the EMJMD in Environmental Contamination and Toxicology (ECT+), with an Erasmus Mundus scholarship (ref: 2019-1485), and Dr. Bernd Nowack, from Empa, Switzerland, for the opportunity to attend the SPSAS NanoAgri&Envi.

Keywords: material flow analysis, titanium dioxide, released nanomaterial, waste management.

Multiple biomarkers in zebrafish (*Danio rerio*) applied to the analysis of ecotoxicity of emerging pollutants in the single health context

L. Pitombeira de Figueirêdo, F.C. Dias, T.L. Rocha
[1] *Federal University of Goiás, Laboratory of Environmental Biotechnology and Ecotoxicology, Institute of Tropical Pathology and Public Health, Goiânia, Brazil*
livia.pitombeira@gmail.com

Since the industrial revolution, many chemicals have been released into the environment. However, in the last 50 years, this release has been even more pronounced [1]. Among these compounds, emerging contaminants, such as drugs, personal care products, hormones, alkylphenols and their derivatives, illicit drugs, nanomaterials, micro(nano)plastics, among others, have been gaining prominence mainly in the last decade. In Brazil, these compounds have already been detected in several aquatic matrices, whether in supply, surface, groundwater and even bottled water, with microplastics being found in a greater number of matrices [2]. Therefore, the present study aimed to evaluate the ecotoxicity of the polyethylene (PE) microplastic through toxicity tests at early development stages (embryos and larvae) of Danio rerio fish, considering multiple biomarkers. For this, a test lasting 144 hours was performed, without solution renewal, in which zebrafish embryos were exposed to concentrations of 0.5, 5.0 and 50 mg PE/L (size = 600□m), and the following endpoints spontaneous contractions, heart rate, hatching rate, survival rate and morphological changes were evaluated. Among the results found, bradycardia was observed, with a significant difference in relation to the control at the highest concentration (50 mg PE/L), as well as a delay in the hatching rate also at this concentration. For the other evaluated criteria, survival, spontaneous movement and morphological alterations, there was no significant difference in relation to the control. Overall, even without lethal effects, it is possible to identify that aquatic organisms may be at risk when exposed to PE due to their sublethal effects during the early stages of development.

[1] NAIDU, R.; BISWAS, B.; WILLETT, I.; CRIBB, J.; SINGH, B.; NATHANAIL, P.; COULON, F.: SEMPLE, K.; JONES, K.; BARCLAY, A.; AITKEN, R. Chemical pollution: A growing peril and potential catastrophic risk to humanity. Environment International. 156. 106616, 2021
[2] MONTAGNER, C. C.; VIDAL, C.; ACAYABA, R. D. Contaminantes emergentes em matrizes aquáticas do Brasil: cenário atual e aspectos analíticos, ecotoxicológicos e regulatórios. Química Nova [online]. 2017, v. 40, n. 9, pp. 1094-1110.
Acknowledgements: This work was supported by Coordination of Superior Level Staff Improvement - CAPES
Keywords: microplastic, polyethene, sub-lethal effects.

Chitosan-alginate edible films to improve fish shelf-life: Development and characterization

Luiz Carlos Corrêa-Filho[1], Jailton Ribeiro Santos Junıor[2], Henriqueta Talita Guimarães Barboza[1], Antônio Gomes Soares[1], Renata Valeriano Tonon[1] and Lourdes Maria Corrêa Cabral[1]
1 Embrapa Food Agroindustry - Rio de Janeiro, Brazil; 2 Federal Rural University of Rio De Janeiro – Rio De Janeiro, Brazil
lucaalbernaz@gmail.com

Some animal products like fishs are highly perishable foods, susceptible to rapid microbiological deterioration during storage. In this way, this work aims to develop active chitosan/alginate films incorporated with zinc oxide (ZnO) nanoparticles, aiming to provide an alternative for preserving and increasing the fish shelf life. Films were produced by casting. The polymer concentration in the filmogenic solutions was 1.5%w/v in the following proportions of alginate:chitosan: 100:0; 25:75; 50:50; 75:25 and 0:100. Chitosan solutions were prepared in 1%v/v aqueous acetic acid under magnetic stirring. The alginate was dissolved in distilled water at 60°C under mechanical agitation at 6,500 rpm. Thereafter, a crosslinking with calcium chloride at 1.0% w/w was performed. In all polymeric solutions, 30%w/w glycerol was added. The polymer solutions were poured in an acrylic plate and dried at 35°C for 48 h. The films were characterized regarding chemical, mechanical and barrier properties. All the evaluated formulations resulted in non-rigid and homogeneous films. Chitosan films were less water soluble than the alginate ones. Elongation and tensile strength values ranged from 3.67 to 17.87% and 16.10 to 37.87 MPa, respectively. It was observed that the increase in alginate concentration led to an increase in the tensile strength and a reduction in elongation at break. Overall, films produced with more than 75% chitosan concentration showed better potential barrier and mechanical properties, mainly low water solubility and higher elongation at break, being suitable for use in formulations intended to produce edible films. It is expected that films with a higher concentration of chitosan have good potential to conduct the study of films incorporated with ZnO nanoparticles.

Acknowledgements: The authors would like to thank CAPES - Higher Education Personal Improvement Coordination (grant #88887.646273/2021-00) and FAPERJ - Fundação de Amparo à Pesquisa do Estado do Rio de Janeiro, Brazil (grant #E-26/204.362/2021).
Keywords: active biopolymer films, antimicrobial activity, zinc oxide

Atmospheric PAH removal by nonwoven fabric filters incorporated with graphene oxide

Manoel Messias Coutinho Meira[1], M. V. Lorevice[2], J. Cristale[1,3], D. S. T. Martinez[1,2] and S. A. Pozza[2]

[1] School of Technology, State University of Campinas, 13484-332, Limeira, Brazil; [2] Brazilian Center for Research in Energy and Materials, Brazilian Nanotechnology National Laboratory, 13083-970, Campinas, Brazil; [3] Center for Nuclear Energy in Agriculture, University of São Paulo, 13400-970, Piracicaba, Brazil.
spozza@unicamp.br

The adverse effects of poor air quality on climate, ecosystems, and human health are well-documented [1]. Among the main atmospheric pollutants, airborne particulate matter (PM) stands out as a significant contributor. PM is associated with respiratory and cardiovascular diseases, increasing significantly mortality rates in affected populations [2]. Due to its high surface area, PM can adsorb various compounds, including polycyclic aromatic hydrocarbons (PAH), which are generated as a product of incomplete combustion of organic matter. The adsorption of PAH by PM particles further contributes to the environmental and health risks associated with poor air quality, as it enhances the potential exposure to these harmful substances. The United States Environmental Protection Agency (EPA) has classified 16 PAHs as priority pollutants due to their carcinogenic and mutagenic properties [3]. The EPA's classification emphasizes the urgency of addressing and mitigating the exposure to these PAHs, as they pose significant threats to both human and environmental well-being. Among the filters available, fibers containing Graphene Oxide (GO) have shown remarkable potential due to their exceptional adsorptive capacity and exhibit a strong affinity for capturing PM [4]. Thus, the project aims to fabricate, characterize, and analyze the filtration efficiency of polypropylene nonwoven fabric (NWF-PP) nanocomposite filters containing GO. The project also aims to evaluate the effectiveness of these filters in capturing the 16 EPA PAHs, thereby assessing the potential for utilizing GO-enhanced filters as a reliable and efficient method for mitigating the presence of these harmful pollutants. GO was applied to the filters by a spray-coating protocol in consecutive drying cycles (1, 2, 5, and 10 cycles), generating a film layer. Scanning electron microscopy (SEM) images suggest that NWF-PP with 5 GO cycles presented superior filtration performance than the other tested cycles and uncovered filters. It is expected a filtration efficiency higher than 95% and a maximum pressure drop of 70 Pa, as well as a high quality factor (QF > 0.7 Pa^{-1}). Furthermore, obtaining a high porosity and permeability filter is desirable for practical applications such as personal protective equipment and domestic filtration.

[1] K. de S. P. Godoi et al., “Mutagenicity in Tradescantia pallida as an Indicator of the Effect of Air Pollution and Human Health,” Atmosphere (Basel), vol. 12, no. 9, p. 1185, Sep. 2021, doi: 10.3390/atmos12091185.
[2] F. Dominici et al., “Fine Particulate Air Pollution and Hospital Admission for Cardiovascular and Respiratory Diseases,” JAMA, vol. 295, no. 10, p. 1127, Mar. 2006, doi: 10.1001/jama.295.10.1127.
[3] EPA. (2014). Priority Pollutant List. https://www.epa.gov/sites/default/files/2015-09/documents/priority-pollutant-list-epa.pdf.
[4] J. Li et al., “Removal of Cu(II) and Fulvic Acid by Graphene Oxide Nanosheets Decorated with Fe3O4 Nanoparticles,” ACS Appl Mater Interfaces, vol. 4, no. 9, pp. 4991–5000, Sep. 2012, doi: 10.1021/am301358b.

Acknowledgments: This study was financed in part by the Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brasil (CAPES) – Finance Code 001. The authors would like to thank the support of the Brazilian Nanotechnology National Laboratory (LNNano) for the use of the internal facilities, and laboratories.

Keywords: adsorption, air filters, particulate matter, polypropylene

Next-Generation Disinfection: Advancements using silver and silicon nanoparticles for a high-performance disinfectant

Marcella C. da Silva[1,2], Robson D. Ferreira[1], Rodrigo B. Nogueira[2], Raiana S. Gurgel[4], Patricia M. Albuquerque[4], and Lizandro Manzato[1,2]

1Instituto Federal de Educação, Ciência e Tecnologia do Amazonas, Laboratório de Síntese e Caracterização de Nanomateriais, Manaus, AM, Brazil.
2Universidade Federal do Amazonas, Manaus, AM, Brazil.
3Universidade Federal de Santa Catarina, Laboratório Interdisciplinar para o Desenvolvimento de Nanoestruturas, Florianópolis, SC, Brazil.
4Universidade do Estado do Amazonas, Escola Superior de Tecnologia, Laboratório de Química Aplicada à Tecnologia, Manaus, AM, Brazil.
**marcella.silva@ifam.edu.br*

The chaotic backdrop of the pandemic has highlighted the importance of containing viral illnesses and fighting the illnesses they cause. In this context, the potential use of nanoscience and nanotechnology approaches demonstrates how these technologies can help technical-scientific communities in combating the pandemic, with emphasis on the development of nanomaterials. Selfinoculation through the mouth, nose, or eyes after touching a contaminated surface in public areas is a potential route of disease transmission. The integration of nanotechnology in commercial disinfection solutions can help in the search for more effective disinfection. The implementation of self-sanitizing surfaces that release antimicrobial actives while exhibiting surface topologies that promote the self-deactivation of viral particles exemplifies how smart surfaces can alleviate the constant and perpetual need for active disinfection. Therefore, not only the disinfection of surfaces but also the use of PPE materials (personal protective equipment), is of utmost importance in controlling the pandemic spread of viruses, including the current SARS-CoV-2. In a typical and simple reaction procedure, nanoparticles (NPs) of Ag and SiO2 were synthesized by the sonochemical method using an ultrasonic purifier (L100 Schuster 42000 Hz), in which an aqueous solution of silver nitrate (1 Mm) was used with an aqueous starch solution and 0.5 mL of sodium silicate solution, respectively. Colloidal suspensions of silver nanoparticles (AgNPs) and silicon dioxide nanoparticles (SiO2NPs) were centrifuged at 6000 rpm for 20 min and washed with distilled water, a process repeated three times. Afterward, the samples were dried by lyophilization. The samples were characterized by FTIR-ATR, XRD, and UV-Vis analysis to identify the biomolecules around the biosynthesized nanoparticles, crystallinity, and their formation, respectively. Afterward, the NPs were incorporated into the formulation of the high-performance commercial disinfectant. The microplate dilution technique was used to evaluate the antimicrobial activity of the biosynthesized NPs, the commercial disinfectant, and the commercial disinfectant with incorporated NPs. Biosynthesized AgNPs did not show activity only against Escherichia coli, Staphylococcus epidermidis, Bacillus subtilis, and Salmonella enterica, while SiO2NPs did not show activity against Staphylococcus aureus, Escherichia coli, Staphylococcus epidermidis, Bacillus subtilis and Enterococcus faecalis.

[1] J. Black and V. White, J. Irrep. Res. 100, 187 (2002).
[2] A. Brown, A. Smith and A. Chemist, The Art of Writing Convincing Abstracts (Pergamon Press, 2000) p 868.

Acknowledgements: We would like to express gratitude to FAPEAM, and CNPq/SisNANO 420601-2019/0 for their valuable support this work possible. Their financial assistance provided the necessary resources for conducting research and achieving significant results.

Keywords: Silver nanoparticles, Silicon nanoparticles, Disinfection, Nanotechnology.

Development of new transparent and transparent chitosan substrates flexible for application in gas sensor devices in the detection of ammonia

Marcos Vinícius Woiski Barcote[1], Maiara de J. B. Gobara[1], Marcelo Eising[1], Helton J. Alves[2], Lucimara S. Roman[1]

1 Universidade Federal do Paraná, Departamento de Fisica, 81531-980, Curitiba, Brazil; 2 Universidade Federal do Paraná, Departamento de Engenharias e Exatas, 85950-000,Palotina,Brazil.
mvwbarcote@gmail.com/mvw.barcote@ufpr.br

Currently, the use of environmentally harmful materials in the manufacture of devices is considered one of the great challenges of electronics, which is why the search for new substrates, in general, has intensified, as well as biodegradable, flexible, and transparent ones. This dissertation has as a product the average molar mass of chitosans (microparticles) and low molar mass (nanoparticles) for application in substrates of gas sensors. In this work, new flexible substrates based on chitosan were developed and different depositions of organic semiconductor materials dispersed in an aqueous medium were studied, such as PEDOT:PSS. Conjugated polymers, dispersed in water and others, constitute a challenge for obtaining thin and homogeneous films, widely used as an active layer in electronic devices. Here, the *slot-die coating* technique was used to deposit reproducible organic chitosan films. For the conjugated polymers, the method used for the deposition of the films was *drop-cast*. The relationship to control the surface and stability of the films, the hydrophobicity of chitosan substrates through wettability, and the optical properties through scanning electron microscopy (SEM) of thin films in which the morphological properties are studied were studied. The mechanical and electrical properties are studied through the bending method, to obtain the resistance to the flexibility of the polymers. These issues are important to produce new organic thin films that can be used in electronic devices. As an application for this work, biodegradable gas sensors for ammonia detection are developed. This work can contribute to the future development of sensors for the detection of ammonia gases, thus expanding the composites' applicability.

[1] Barcote, M. V. W. (2023). Desenvolvimento de novos substratos de quitosana transparentes e flexíveis para aplicação em dispositivos sensores de gás na detecção de amônia (Dissertação Digital Mestre). Universidade Federal do Paraná. Retirado de http://hdl.handle.net/1884/82361 J. Black and V. White, J. Irrep. Res. 100, 187 (2002).

Acknowledgements: The authors acknowledge the research funding from CAPES, CNPq, and COPEL.

Keywords: Chitosan, thin film, biodegradable, ammonia gas sensing.

Synthesis and Structural Properties of Graphene Oxide for the Production of Biocompatible Films with Antibiofilm Action

Silva M.E.C.M.[1], Ribeiro F.A.S.[1], Arruda I.RS.[2], Silva R.C.S.[2], Santos L.R.L.[2], Machado G.[2]
1Universidade Federal de Pernambuco, Departamento de Ciência de materiais, 50670-901, Recife, Brazil; 2 Centro de Tecnologias Estrategicas do Nordeste, Nanotecnologia, 50740-545, Recife, Brazil.
maria.mesquita@cetene.gov.br

One of the major challenges in the biomedical industry is bacterial adhesion, which can lead to product malfunction and widespread infections in the host. The most commonly used approach to mitigate these damages is coating the material to achieve a surface that prevents bacterial attachment. This coating can be done using metallic nanoparticles or organic polymers. Nanoparticles, when compared to conventional antibiotics, offer certain advantages such as low toxicity, overcoming microbial resistance, and reduced costs. In recent years, research on the graphene family has been at the forefront of the biomedical sector, with a focus on its synthesis [1]. The most widely used method for obtaining graphene oxide (GO) is the Hummers-Offerman approach, which involves the oxidation and exfoliation of graphite [2]. In this work, the synthesis of antibiofilm GO is proposed for the subsequent functionalization of ear extenders. For this purpose, the synthesis of graphene oxide, the main active component of the research, followed the modified Hummers-Offerman method, where graphite was added to an ice bath under agitation along with potassium permanganate. Subsequent addition of concentrated sulfuric acid was performed to remove impurities, followed by centrifugation of the material and exchange of the supernatant to achieve a pH close to neutral. Analysis of graphite, graphene oxide, and reduced graphene oxide was conducted. The number of layers was determined through X-ray diffraction (XRD) analysis, with 102 layers for graphite and 11 layers for graphene oxide, a known limit for identifying the formation of GO. The chemical composition was obtained through Raman and FTIR spectroscopy correlated with thermal analysis by thermogravimetry (TG) to determine the physicochemical characteristics of the material. The morphology of GO was examined using Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM), revealing the presence of characteristic GO layers. In the thermal analysis, graphite exhibited high thermal stability without any significant mass loss between 100°C and 900°C, unlike graphene oxide, which showed a peak near 180°C, indicative of the loss of functional groups and confirming the formation of the compound. For antibacterial and antibiofilm analysis, broth microdilution was performed using a 96-well plate, testing the bacteria Staphylococcus epidermidis and Escherichia coli. Satisfactory results were obtained at low concentrations of GO against E. coli biofilm formation, inhibiting over 50% of its growth. GO exhibits high potential for the development of biocompatible films with antibiofilm activity.

[1] MANDAL, P.; Ghosh, S.K.; Grewal, H.S. Graphene oxide coated aluminium as an efficient antibacterial surface. Environmental Technology & Innovation. 28 (2022)
[2] Priyadarsini, S.; Mohanty, S.; Mukherjee, S.; Basu, S.; Mishra, M. Graphene and graphene oxide as nanomaterials for medicine and biology application. Journal of Nanostructure in Chemistry v.8, 123–137, 2018.

Acknowledgements: This work was supported by Ministério da Ciência e Tecnologia (MCTI), Centro de Tecnologias Estratégicas do Nordeste (CETENE), Fundação de Amparo à Ciência e Tecnologia de Pernambuco (FACEPE) and CNPq.

Keywords: Graphene oxide, biocompatibility, stenosis, biofilm

Toxicological evaluation of silver nanoparticles obtained by green synthesis in *Caenorhabditis elegans*

Maria Eduarda Oliveira de Souza[1], H. A. Padilha[1], A. C. D. Filho[2], E. L. G. Denardin[2] and D. S. de Ávila[1]

1 Universidade Federal do Pampa, Programa de pós-graduação em bioquímica, Grupo de Pesquisa em Bioquímica e Toxicologia em C. elegans, Uruguaiana, Brazil; 2 Universidade Federal do Pampa, Laboratório de Química de Produtos Naturais, Uruguaiana, Brazil.

mariaeduarda.aluno@unipampa.edu.br

The use of nanoparticles is becoming more recurrent, being widely used from technological applications in chips, cell circuits and computers to the biomedical area as in stents and pacemakers. This is due to its optoelectronic properties directly related to its quantum size and *bulky scale*. Therefore, it is necessary to carry out studies evaluating their toxicity, provide the biosafety of the application of these materials at the nanoscale, based on alternative animal models. The objective of this work was to evaluate the toxicity of silver nanoparticles (AgNPs) obtained through green synthesis with *Bougainvillea glabra Choisy* extract (BgC), using light from Light Emitting Diodes as a catalyst, at different wavelengths. As an *in vivo* experimental model, *Caenorhabditis elegans* was chosen, a free-living nematode, widely used for toxicological tests, which in addition to being compatible with the principles of the 3R's (reduce, replace and refine), has a genetic homology of about 80% with the mammals. To obtain AgNPs, a silver nitrate solution (AgNO3, 1 mmol.L-1) and BgC extract were used, and the mixture was incubated in a box coated inside with LED light, emitting the colors white, red and violet (in independent processes) as a catalyst under stirring for 24 hours. At the L1 larval stage were exposed and divided into a control group (exposed only to H2Od) and groups treated with AgNPs White, Violet and Red (0.1; 1; 5; 10 µg.mL-1) in liquid medium for 30 minutes (acute treatment). From there, the worms were poured into Petri plates with NGM medium (growth medium for nematodes) with *E. coli OP50* (food source) and remained for 48 hours in the incubator at 20°C. With the animals in the L4 larval stage, the following parameters were performed: survival rate, quantification of body area and brood size. It was possible to observe a high rate of toxicity with a significant decrease in the survival of the worms, except for the concentration of 0.1 µg.mL-1, which proved to be safe. From this, the LC50 was determined, which was respectively 0.5427, 0.6345 and 0.5979 µg.mL-1 for AgNPs synthesized with White, Violet and Red light as catalysts. All groups treated with AgNPs at a concentration of 0.01 µg.mL-1 showed no significant difference in body area when compared to the control group. In the parameter that evaluates the reproduction of the worms, both concentrations tested (0.1 and 1 µg.mL-1) of the three groups (White, Violet and Red) did not show significant changes in the number of progeny. According to these findings, it was verified that the AgNPs were toxic in most of the tested concentrations (0,1; 1; 5; 10 µg.mL-1), presenting a possible anthelmintic action. To evaluate its mechanism of action, further tests such as quantification of the expression of antioxidant enzymes and evaluation of nematode locomotion will be carried out.

Acknowledgements: This work was supported by Coordenação de Aperfeiçoamento de Pessol de Nível Superior (Capes) and Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq).

Keywords: silver nanoparticles, C. elegans and toxicity.

Nanocarriers labeled with gold nanoparticles: a potential strategy to understand the interaction of nano-enabled agrochemical in plants

M. M. L. Forini[1], D. R. Antunes[1], L. A. F. Cavalcante[1], M. S. Pontes[2], E. F. Santiago[2], A. O. Sanches[1], A. R. Martins[3], R. Grillo[1*]

1 São Paulo State University UNESP), Department of Physics and Chemistry, Faculty of Engineering, Ilha Solteira, SP, Brazil. 2 Center for Natural Resources Study (CERNA), Mato Grosso Do Sul State University (UEMS), Dourados, MS, Brazil. 3 São Paulo State University (UNESP), Department of Biology and Zootechnics, Faculty of Engineering, Ilha Solteira, SP, Brazil.

renato.grillo@unesp.br and mariana.forini@unesp.br

Engineered nanoherbicides have recently been developed to control pests and promote more sustainable agriculture. Such nano-enabled materials have shown unique properties [1] for agricultural purposes since they can control the release of active ingredients in the field and promote better efficiency control in weeds compared to conventional herbicides. However, studies on the fate, behavior, and mechanism of action of lipid nanoherbicides in plants are still incipient. In this study, nanostructured lipid carriers, already used as nanoherbicides, were labeled with gold nanoparticles to investigate their fate in aquatic macrophytes (*Lemna valdiviana*). Thus, nanostructured lipid carriers labeled with gold nanoparticles were prepared by the emulsification/solvent evaporation method and characterized by different physicochemical techniques. Scanning electron microscopy showed spherical morphology with a size distribution between 200 and 250 nm. Transmission electron microscopy analysis indicated that the nanocarriers presented a well-defined core-shell structure, in which the gold nanoparticles presented an average size of 11 nm. Also, the encapsulation efficiency value of Au NPs in the nanostructured lipid carrier was 99.94%. The release profile of gold ions showed a low dissociation rate since only 0,15% of gold ions were free in the solution for approximately 6 days. The techniques of infrared spectroscopy (FTIR), X-ray diffraction (XRD), atomic absorption spectroscopy, and optical microscopy revealed the internalization of hybrid nanocarriers in the aquatic plants, which depends on the concentration and exposure time. Therefore, this study can contribute to understanding the mechanism of action and the future design of new “safe-by-design” nanopesticides.

[1] Wang, D., Saleh, N. B., Byro, A., Zepp, R., Sahle-Demessie, E., Luxton, T. P., Ho, K. T., Burgess, R. M., Flury, M., White, J. C., Su, C. Nature Nanotechnology. 17 (4), 347-360 (2022).
[2] Takeshita, V., Carvalho, L. B., Galhardi, J. A., Munhoz-Garcia, G. V., Pimpinato, R. F., Oliveira, H. C., Tornisielo, V. L., Fraceto, L. F. ACS Nanoscience Au. 2 (4), 307-323 (2022).

Acknowledgments: The authors would like to thank São Paulo Research Foundation (Grants #2017/21004 5, #2019/20124-2, #2020/12769-0), National Council for Scientific and Technological Development (Grant #427498/2018-0, #161360/2021-1) and Coordenação de Aperfeiçoamento de Pessoal de Nível Superior – Brazil, CAPES – Finance Code 001.

Keywords: nanoherbicides, tracking, gold nanoparticles, Lemna valdiviana.

Predicting electrophoretic mobility of TiO_2, ZnO, and CeO_2 nanoparticles in natural waters: The importance of environment descriptors in nanoinformatics models

Marta Swirog[1], Alicja Mikolajczyk[1], Tomasz Puzyn[1]
[1] QSAR Lab, Gdansk Science and Technology Park, Trzy Lipy 3 Street, 80- 172 Gdansk, Poland.
t.puzyn@qsarlab.com

Natural and engineered nanoparticles (NPs) entering the environment are influenced by many physicochemical processes and show various behavior in different systems (e.g., natural waters showing different characteristics). Aggregation is an essential process for the transport and fate of NP in natural waters, and changes in the aggregation state cause alterations in the exposure of living organisms to NPs and their uptake. This leads to different biological and ecotoxicological effects and drives attention to the need for NPs risk assessment for the environment [1]. Experimental methods provide extremely useful data, but quantitative structure-property relationships (QSPR) modeling is an indisputably cheaper, less time-consuming, and safer way of predicting NPs properties. For a long time, researchers have considered NPs' behavior and mechanisms of action mainly due to their structure, developing descriptors that comprehensively describe NP and predict their properties (endpoints) of interest [2]. However, one should ask oneself, since the natural environment is such a dynamically changing system, is it appropriate to base the predictions only on the characteristics of the NP? I hypothesized that the most effective way to predict changes in environmental fate-relevant properties of NPs is to use a combination of descriptors of nanoparticles' structure and descriptors of the environment. My research assumes that instead of utilizing descriptors of NPs 'structure as the only input for the model, in parallel, two blocks of information should be used: the NPs' structure descriptors and the environment descriptors. Thanks to this, the model could consider the actual influence of the medium's conditions on the behavior of the NP. The types of environments can be viewed through the prism of the NP life cycle- from production, through a presence in the natural environment, to entering a living organism. As a proof-of-the-concept, I have developed a group of models (including MLR, GA-PLS, PCR, and Meta-Consensus models) with high predictive capabilities (Q_{EXT2} = 0.931 for the GA-PLS model), where the S-descriptors are represented by the core-shell model descriptors [3], and the E-descriptors – by different ambient water features (including ions concentration and the ionic strength). The newly proposed nano-QSEPR modeling scheme can be efficiently used to design safe and sustainable nanomaterials and it gives an overview of the importance of environmental parameters over the NP structure and the possible bioavailability of NPs to living organisms. Further research envisages the development of applied methodology and testing model universality concerning other environments.

[1] S. M. Louie, R. Ma, and G. V. Lowry, Frontiers of Nanoscience, vol. 7, pp. 55–87 (2014).
[2] S. Kar, A. Gajewicz, T. Puzyn, K. Roy, and J. Leszczynski, Ecotoxicology and Environmental Safety, vol. 107, pp. 162–169(2014)
[3] K. Tämm et al., Nanoscale, vol. 8, no. 36, pp. 16243–16250 (2016).

Acknowledgements: This work has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No. 814426 (NanoInformaTIX project).

Keywords: nano-QSPR, environment, aggregation, zeta potential

Evaluation and characterization of silver nanoparticles synthesized by the 'green synthesis' method using seaweed from the coast of Pernambuco as reducing agentes

Matheus Alves Siqueira de Assunção[1], Douglas Dourado[1], Leonardo Gabriel Cabral de Melo Souza[1], Mara Elga Medeiros Braga[2], Severino Alves Júnior[3], Fábio Rocha Formiga[1]

1 Aggeu Magalhães Institute (IAM), Oswaldo Cruz Foundation (FIOCRUZ), 50670-420 Recife, PE, Brazi; 2 University of Coimbra, CIEPQPF, Department of Chemical Engineering, Rua Sílvio Lima, Pólo II – Pinhal de Marrocos, 3030-548 Coimbra, Portugal; 3 University Federal of Pernambuco, Department of Chemistry, Laboratório de Terras Raras, 50590-470, Recife, Brazil. matheus.alves.dfj@hotmail.com

Introduction: The biosynthesis of metallic nanoparticles from natural extracts has been proposed as a new alternative methodology, in which the constituents of the extracts act as reducing agents and stabilizers of the nanoparticles, so that this approach can explore the synergistic larvicidal potential between the nanoparticles and the bioactive compounds present in the extracts [1]. **Objectives**: The objectives of this study were to investigate a cheap and nature-friendly method for the formation of silver nanoparticles (AgNPs) using algae as a reducing agent and to characterize the AgNPs. **Methods**: Seaweeds were collected on Serrambi beach, Ipojuca, Pernambuco, Brazil, dried and used for the preparation of crude extracts. Silver nanoparticles (AgNPs) were prepared by green synthesis using 1mM silver nitrate (AgNO3) and crude seaweed extract in a reaction mixture. AgNPs were characterized by UV-vis, DLS, Zeta Potential and TEM. **Results**: All seaweed aqueous extracts were able to reduce silver salt and form AgNPs, showing UV-vis peaks between 400 and 430nm. The values found are similar to the values found by Sinha et al. (2015) [2], where they demonstrated that the production of AgNPs using the green alga presented a peak at 445nm that indicates a surface plasmonic resonance (SPR), which has already been recorded for several metallic nanoparticles that varied from 2 to 100 nm in size [2, 3]. The values obtained by the DLS technique in a polydisperse mixture, showed sizes ranging from 45.81 to 234.9, as well as the values of the Polydispersion Index (PdI), ranging from 0.305 to 0.522, corroborating the findings by Bonatto and Silva (2014) [4], which indicate that silver nanoparticles formed by green synthesis routes will generally have a moderate PdI, ranging between 0.3 and 0.5 [4]. All suspensions obtained showed negatively charged zeta potential in aqueous medium, with values ranging from - 29.7 to -36.0. TEM analyzes demonstrated spherical nanoparticles both isolated and aggregated, containing particles ranging in size from 20 to 150nm. **Conclusions**: The aqueous extracts of the selected algae were effective in the formation of AgNPs, showing reducing and stabilizing capacity demonstrating potential applications in the biomedical field and this simple procedure has several advantages, such as cost-effectiveness and compatibility for biomedical and pharmaceutical applications.

[1] Vimala, R.; Sathishkumar, G.; Sivaramakrishnan, S. J. S. A. P. A. M.; SPECTROSCOPY, B. Optimization of reaction conditions to fabricate nano-silver using Couroupita guianensis Aubl.(leaf & fruit) and its enhanced larvicidal effect. 135, p. 110-115, 2015.
[2] Sinha, S. N.; Paul, D.; Halder, N.; Sengupta, D. et al. Green synthesis of silver nanoparticles using fresh water green alga Pithophora oedogonia (Mont.) Wittrock and evaluation of their antibacterial activity. 5, n. 6, p. 703-709, 2015.
[3] Ravindra, B.; Rajasab, A. A comparative study on biosynthesis of silver nanoparticles using four different fungal species. 2014.
[4] Bonatto, C. C.; Silva, L. P. Higher temperatures speed up the growth and control the size and optoelectrical properties of silver nanoparticles greenly synthesized by cashew nutshells. Industrial Crops and Products, 58, p. 46-54, 2014/07/01/ 2014.

Acknowledgements: This work was supported by FACEPE.

Keywords: Silver nanoparticles; Green synthesis; Macroalgae; Crude extract

Design and optimization of automated systems for studying ionic transport in Graphene Oxide membranes for water purification

Matheus Santos Dias[1,2], Edvaldo Angelo[1] and Camila Marchetti Maroneze[1,2]
1 Mackenzie Presbyterian University, Engineering School, 01302-907, São Paulo, Brazil; 2 Mackenzie Institute for Research in Graphene and Nanotechnologies (MackGraphe).
camila.maroneze@mackenzie.b
r

Ionic and molecular sieving using membranes with subnanometer pores has attracted the widespread interest of the scientific community due to the broad applications in industrial processes such as water purification and desalination, energy conversion, sensing, and other important separation technologies. The two-dimensional (2D) materials like graphene and its derivatives, transition metal dichalcogenides (TMDs), MXenes, and mineral clays are promising nanostructures that can be exfoliated into single- or few-layered nanosheets and reassembled into functional membranes with tunable size and porosity. Special attention has been given to graphene oxide on account of its tunable physicochemical properties and more realistic prospects for industrial-scale production. The current methods for the development and study of the performance of new membranes for water purification on a laboratory scale still endure high operating costs due to the instrumentation required and the time-consuming routine involved in real-time monitoring of the separation process. This work presents the development of a methodology for the study of 2D lamellar membranes (47 mm in diameter) composed by three different low-cost, miniaturized, and automated systems of assessment: (1) a 3d printed static ionic diffusion device without applying additional pressures with water conductivity monitoring; (2) a forward osmosis cell fabricated with acrylic and 3d printed parts, monitored by the variation in the level of the fluids separated by the membrane and a (3) acrylic based fluidic filtration system by tangential flow to the membrane surface under high pressure based on reverse osmosis conditions. The devices configurations were designed using CAD software (Autodesk Fusion 360) and fabricated in a desktop CNC milling machine and a 3d printer with PETG filament. Two different proposals have been tested using the fabricated devices: (i) graphene oxide membranes for the separation of ionic species (NaCl) in water and (ii) vermiculite membranes for oil-water separation. In the first case, the three systems were used in parallel where the conductivity of the permeate (apparatus 1, 3) and water level variation (apparatus 2) were used to monitor the performance of the membranes in terms of permeability and salt rejection. For oil-water separation, the apparatus 3 was used and the efficiency of the membrane was studied by spectrophotometric analysis of the permeate. The operation of the reverse osmosis system was tested in the 1 – 20 bar pressure range. The systems showed excellent stability, operating continuously for more than 168 hours, without any type of leakage, both in ionic diffusion, forward osmosis, and reverse osmosis processes for the separation of ionic species and the separation of water-oil emulsion. Furthermore, the structure of the devices proved to be fully compatible with the surfaces of membranes based on 2D materials, not inducing any type of mechanical damage to the membranes. Based on our preliminary results, miniaturized electrochemical sensors and cameras assisted by machine learning can be integrated into the systems, allowing us to perform the real-time monitoring of the separation process, in a simple, fast, and robust way.

Acknowledgements: This work was supported by Petrobras and MackPesquisa.

Keywords: Water treatment, 2D materials, Lamelar membranes.

Cannabis extract-loaded lipid and chitosan-coated lipid nanoparticles with antifungal activity

Matías Menossi[1], G. Tejada[1], S.L. Colman[2], D. Nercessian[2], J.R. Mendieta[2] and V.A. Alvarez[1]
[1] Universidad Nacional de Mar del Plata (UNMdP), Instituto de Investigaciones en Ciencia y Tecnología de Materiales (INTEMA), 7600, Mar del Plata, Argentina; [2] UNMdP, Laboratorio de Genética, 7600, Mar del Plata, Argentina.
matiasmenossi@conicet.gov.ar

The excessive and indiscriminate use of agrochemicals and toxic fumigants play a key role in the maximization of agricultural production worldwide. Despite their benefits, they produce environmental pollution, increasing pesticide/herbicide resistance and destruction of beneficial insects, and placing the health of producers and consumers at risk. This scenario has enabled the development of new scientific approaches focused on eco-friendly alternatives and safer forms of pest management including the use of botanical products such as plant extracts and essential oils with insecticidal action. Nanotechnology has shown promising potential to provide smart tools and materials in order to contribute to agriculture and, in particular, to this eco-friendly perspective. In fact, the application of nanotechnology in agriculture sector goals is double: 1) maximizing food production in a safe, sustainable, and efficient way, with higher food nutritional value; and 2) improving the use of water, light and agrochemicals [1]. Among these smart nano-sized formulations, nano-pesticides represent an effective and sustainable pest management. Nano-based materials can be composed of inorganic and/or organic structures, and they can include or load with specific active ingredients (AIs) [2]. Cannabis resin was obtained from female inflorescences of Cannabis sativa plants belonging to the collection of cannabis biology group; and according to the HPLC characterization study, the cannabis extract used was composed by 770.3 mg (tetrahydrocannabinol (THC)), 72.1 mg (cannabidiol (CBD)) and 28.6 mg (cannabinol (CBN)) per mg cannabis resin. Lipid nanoparticles (NPL) containing cannabis extract were synthesized by homogenization with the ultrasonication method into a matrix composed of cetyl palmitate (CP) coated with chitosan (Q). Briefly, 400 mg of lipid (2.0% w/v) was melted at 60 °C in a water bath, followed by the addition of 500 µL of C extract. The C extract was previously dissolved in ethanol (0.034 mg/mL). Meanwhile, a thermostatized aqueous solution (20 mL) containing 3.0 % w/v F68 was prepared and then added to the melted lipid phase. Immediately, the mixture was sonicated at 65% amplitude for 10 min with an ultrasonic homogenizer (Cole-Parmer 750-W, USA) equipped with a 6 mm titanium tip. Finally, the dispersion was cooled at room temperature and stored at 5 °C. For the preparation of the Q-coated NPL (NPLQ) and NPLQ with C extract (NPLQC), the same protocol was followed but changing the aqueous phase with 3.0 % (w/v) to F68, and 0.2% (w/v) Q. Dry powders of the formulations were obtained by freeze-drying. The NPL formulations were characterized by dynamic light scattering (DLS) and field emission scanning electron microscopy (FE-SEM), showing a spherical morphology in the range of 150 – 240 nm with low polydispersity indexes. Entrapment efficiency of cannabis was higher than 20% and effectively in vitro released in 360 minutes. The NPL formulations were characterized by thermal analysis (DSC and TGA), chemical microstructure (FT-IR) and crystalline structure (XRD). Particularly, the Q-coated NPL formulation loaded with cannabis was effective in inhibiting *Fusarium solani* sp. Eumartiis pores. These results suggesting that the developed NPL system is a safe and good potential candidate for the selective delivery with antifungal activity.

[1] G.V. Lowry, A. Avellan, L.M. Gilbertson, Nat. Nanotechnology, 14, 517-522 (2019)
[2] M. Menossi, R.P. Ollier, C.A. Casalongué, V.A. Alvarez, J. Chem. Technol. Biotechnol., 96, 2109-2122 (2021).
Acknowledgements: This work was supported by grants from Consejo Nacional de Investigaciones Científicas y Técnicas de la República Argentina (CONICET) (PIP 0617), Agencia Nacional de Promoción de la Investigación, el Desarrollo Tecnológico y la Innovación (Agencia I+D+i) (PICT2020-SERIE A-02207). The authors would like to thank Andrés Torrres Nicolini (UNMdP/INTEMA) for helping us in this work.
Keywords: nanoparticles; lipid; chitosan; cannabis.

Enhancing Photocatalytic Degradation of Textile Effluents Using g-$_3N_4$/$CoMoO_4$ Nanocomposites

Mayra L. G. Rodrigues[1], Isabelle M. D. Gonzaga[1], Lara K. Ribeiro[1], Juan Andrés[2], Lucia H. Mascaro[1], Elson Longo[1] e Marcelo Assis[2]

1 Center for Functional Materials Development (CDMF), Federal University of São Carlos (UFSCar), São Carlos, Brazil. 2 Department of Physical and Analytical Chemistry, University Jaume I (UJI), Castelló, Spain.

mayrarodrigues@estudante.ufscar.br

Unleashed industrial growth and the increasing global population in recent years are the main factors contributing to environmental pollution.[1] Therefore, to ensure sustainable and long-term development of human society, there is an urgent need for the development of environmentally friendly and renewable technologies for environmental remediation.[2] Among the various proposed technologies, semiconductor-based photocatalysis holds great potential as it directly utilizes solar energy for the production of valuable chemical fuels and the degradation of harmful pollutants.[3] In this study, g-C_3N_4/$CoMoO_4$ nanocomposites are proposed as catalysts for the photocatalytic degradation of real effluents from the textile industry. The materials were analyzed using X-ray diffraction, Raman spectroscopy, diffuse reflectance spectroscopy, and scanning electron microscopy, confirming the formation of the heterostructure. In the photodegradation tests under UV light, it was observed that g-C_3N_4 outperformed the proposed nanocomposites in the discoloration of the standard RhB molecule. However, for the degradation of the real effluent, it was observed that the mineralization power of the nanocomposite increased by 40% compared to g-C_3N_4, proving that this strategy is more efficient for the mineralization of real textile effluent. This process is attributed to the better separation of the photo-generated charges occurring in the nanocomposite, thus preventing their recombination.

[1] D. Tong, Q. Zhang, Y. Zheng, K. Caldeira, C. Shearer, C. Hong, Y. Qin, S. J. Davis, Nature, 2019, 572, 373–377.
[2] R. Shen, J. Xie, Q. Xiang, X. Chen, J. Jiang, X. Li, Chin. J. Catal., 2019, 40, 240–288.
[3] M. R. D. Khaki, M. S. Shafeeyan, A. A. A. Raman, W. M. A. W. Daud, J. Environ. Manage., 2017, 198, 78–94.

Acknowledgements: This work was partially funded by the São Paulo Research Foundation - FAPESP (2013/07296-2, 2022/09715-1). L. K. R. was supported by SHELL (5333.1). (M.A was supported by Margarita Salas MGS/2021/21 (UP2021-021) grant funded by the European Union Next Generation-EU program.

Keywords: photocatalysis, heterojunctions, CoMoO4, g-C3N4.

The nano-QSPR model for classifying ENM solubility in the natural aquatic Environment

Michal Kalapus[1], T. Puzyn[1,2]
[1] *University of Gdansk, Faculty of Chemistry, Laboratory of Environmental Chemometrics, Wita Stwosza 63, 80-308 Gdansk, Poland;* [2] *QSAR (Quantitative Structure-Activity Relationship) Laboratory Limited, Aleja Grunwaldzka 190/102, 80-266 Gdansk, Poland.*
michal.kalapus@ug.edu.pl

Previous studies show that ENMs can be very toxic to living organisms [1]. Heavy metal ions'effects on living cells are among the main toxicity mechanisms [2]. Thus, the solubility of ENMs in different environmental matrices should be considered in assessing toxicity. Therefore, to better understand the life cycle of nanoparticles (NPs) and the dissolution process in the environment, we must consider that system changes in time, from both the properties of ENM and medium. So, we are looking for an answer to the question: how to predict the solubility of ENMs in a dynamically evolving system? To further clarify the solubility process for 115 metal nanoparticles and nano metal oxides, a set of experimental solubility data collected from the literature was prepared. Then, based on OECD guidelines, the nanoparticles were grouped into two, three or four classes based on their solubility under given conditions. Classification models were made using Decision Trees (DT), Random Forests (RF), Gradient Boosting (GB) and Extra Trees (ET) methods to predict which class the compounds would belong to. The models were trained using data collected at an earlier stage, and external validation was performed. The accuracy score for the validation sets ranges from 0.89 to 1, depending on the model type. This research aimed to predict the solubility of ENMs in water and understand the influence of nanoparticle features and environmental factors. As shown in this work, we can assess with high accuracy, which solubility class in a specific medium ENM belongs to. Moreover, when the composition of the environment or nanomaterials changes, we can estimate with the use of nano-QSPR models whether nanoparticles move to the other class. The study found that ENM solubility is affected by intrinsic nanomaterial properties and extrinsic factors such as pH, organic matter, and ionic strength. Binary models had better predictive power overall, while multiclassification models provided more detailed information on solubility. These models can aid in risk assessment and regulatory decision-making. Future studies should consider additional factors like dissolved oxygen and specific ions.

[1]J. Wang et al.,"Toxicity of zinc oxide nanoparticles to zebrafish embryo: a physicochemical study of toxicity mechanism," vol. 12, no. 5, p. 1645, Jun. (2010), doi: 10.1007/s11051-009-9740-9.
[2] V. Aruoja, H.-C. Dubourguier, H.-C. Dubourguier, K. Kasemets, and A. Kahru, "Toxicity of nanoparticles of CuO, ZnO and TiO2 to microalgae Pseudokirchneriella subcapitata," Science of The Total Environment, Feb. (2009), doi: 10.1016/j.scitotenv.2008.10.053.

Acknowledgments: This research was funded by National Science Centre, Poland [Grant number: UMO-2020/39/B/ST5/02497]. Computations were carried out using the computers of Centre of Informatics Tricity Academic Supercomputer & Network.

Keywords: solubility, nano-QSPR, environment

Synthesis and characterization of zinc oxide (ZnO) and ZnO doped with divalent cations (Mg, Ca) and its evaluation on the concentration of environmental pollutants in water sources

Monica Andrea Vargas[1,2], Jesus E. Diosa[1,3] and Jorge E. Rodríguez[2]
[1] Transiciones de Fase y Materiales Funcionales- Universidad del Valle, Cali, Colombia; [2] Ciencia y Tecnología de Materiales Cerámicos CYTEMAC- Universidad del Cauca, Popayán, Colombia; [3] Centro de Excelencia en nuevos materiales CENM - Universidad del Valle, Cali, Colombia.
monicavargas@correounivalle.edu.co

Zinc oxide (ZnO) is a semiconductor that has generated great interest in recent years due to its physical properties. These include optical properties. The optical properties have been widely studied and ZnO is currently considered an optoelectronic material with very promising qualities for used in numerous technological applications. The structural, morphological and optical characteristics of these materials can be modified depending on the synthesis method, in addition to the concentrations of dopant that enter the structure. Synthesizing by means of a chemical method makes it possible to carry out the synthesis of porous materials, which, by incorporating nanoscale porosity, alter their properties due to the increase in the specific surface area of the structures. This permits an increase in surface chemical reactivity, making these structures attractive in energy applications due to their ability to absorb and interact with species on their surface. Meanwhile, different types of pollution affect the air, soil and water. In this study, only pollutants of water will be considered. Water pollution not only generates physical or aesthetic problems in the affected bodies of water, i.e. in rivers and underground streams, lakes, estuaries and even the sea: it transcends the field of environmental and human health. Human communities need to make use of a number of surface water resources to supply themselves with water, for example to drink. If these are contaminated, it could result in serious epidemiological problems. In addition, environmental problems may be generated since water is a scarce commodity that has been used intensively and irresponsibly in recent decades. Due to their physicochemical characteristics, nanoparticles of different metal oxides have been evaluated both in water purification and in the removal of dyes, bacteria, fungi and, in general, polluting organic molecules, showing great potential in environmental remediation. As such, the project aims to obtain ceramic nanoparticles of zinc oxide (ZnO NPs) and ZnO doped with MgO/CaO in different proportions, using the polymeric precursor method. A simple, reproducible methodology was structured that allowed nanoparticles of the aforementioned systems to be obtained in a controlled manner and with good chemical purity. This method that allowed it possible to obtain particles with a nanometric size, a property that that determine the final characteristics of the product. The synthesized solids were suitably characterized, from the structural, optical and morphological point of view using different techniques, considering their potential application in environmental remediation. Once the ceramic powders have been obtained, they dispersed in aqueous solutions containing environmental pollutants such as dye, an agrochemical, and in water designed with predetermined pollutants, to evaluate the effect of removal of the synthesized nanoparticles on the concentration of pollutants. The results obtained from this research will be of interest to the field of environmental remediation since they would allow, with their application, to reduce the pollutant load contained in wastewater. In addition, with this research, information obtained that, in the future, could allow working on the design of prototypes of water treatment plants using nanotechnology, an action aimed at preserving the environment.

Keywords: Polymer precursor, ZnO, dopants, methyl orange.

Synthesis and characterisation of WS_2

M. A. Ballim, N. Moloto[1]
[1] *Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private bag 3, WITS, 2050, Johannesburg, South Africa.*
0708602k@students.wits.ac.za

Transition metal dichalcogenides (TMDs) are layered materials having a metal between two chalcogens (X-M-X) which have unique properties [1]. Among these TMDs, Tungsten disulfide (WS_2), a 2D, layered structure, has good thermal stability, a high surface area, high carrier mobility and tunable band structure. There is also strong polar X-S covalent bonds at the lamellar layers' edges that can attract polar species. [2] WS_2 has been used in lithium-ion batteries, lubricants, sensors, photonic devices, and water purification. [3] It is usually synthesized via hydrothermal technique, chemical vapor deposition (CVD) and liquid-phase exfoliation (LPE) which provides an array of nanostructures. WS_2 was synthesized using the colloidal synthesis method where the capping agents were varied. This method allows for mild conditions, reaction parameters that are variable and the possibility to scale up. [4] The capping agent determines the morphology and size of the nanoparticles. [4] Multi-layer WS_2 was synthesized due to the presence of the (002) plane observed in the X-ray diffractogram. [5] WS_2 nanoflowers were observed in transmission electron microscopy (TEM) when the capping agents octadecene, oleic acid and oleyl amine were used. The capping agent oleyl amine alone produced a closed flower structure while oleyl alcohol produced nanosheets.

[1] W. Choi, N. Choudary, G. H. Han, J. Park, D. Akinwande, Y. H. Lee, Mater. Today, 20, 116 (2017)
[2] G. Li, Y. Wang, J. Bi, X. Huang, Y. Mao, L. Luo and H. Hao, Nanomaterials, 10, 278 (2020)
[3] A. Yousef, Z. Thiehmed, R. A. Shakoor and T. Altahtamouni, Catalysts, 12, 1138 (2022)
[4] S. L. Mphahlele, Colloidal synthesis of WS2 nanostructures for applications as electrode materials (University of the Witwatersrand, 2019) p 4
[5] S.S. Gqoba, Synthesis, characterization and application of 2D semiconducting layered inorganic nanostructures of In2S3 and WS2 in gas sensing (University of the Witwatersrand, 2018) p 46

Acknowledgements: This work was supported by the National Research Foundation (NRF) South Africa. The authors would like to thank NRF, WITS, CATMAT, NANOWEBS, SPSAS.

Keywords: Nanomaterials, Tungsten disulphide, Colloidal synthesis.

Raman Spectroscopic analysis of human serum samples of convalescing COVID-19 positive patients

N. Jackson[1], J. Hassan[2] and H.J.Byrne[1]
1FOCAS Research Institute, TU Dublin, City Campus, Dublin 8, Ireland
2National Virus Reference Laboratory, University College Dublin, Belfield, Dublin 4, Ireland
Naomi.jackson@tudublin.ie

Rapid screening, detection and monitoring of viral infection is of critical importance, as exemplified by the rapid spread of SARS-CoV-2, leading to the worldwide pandemic of COVID-19. This is equally the case for the stages of patient convalescence as for the initial stages of infection, to understand the medium and long terms effects, as well as the efficacy of therapeutic interventions. Optical spectroscopic techniques potentially offer an alternative to currently employed techniques of screening for the presence, or the response to infection. In this study, the ability of Raman spectroscopy to distinguish between samples of the serum of convalescent COVID-19 positive patients and COVID-19 negative serum samples, and to further analyse and quantify systemic responses, was explored. The study included serum samples of patients who had been tested for SARS-CoV-2 specific IgG and IgM responses between 25 and 134 days after the infection was identified. Both COVID-19 positive and negative groups included males and females who ranged in age from 21 to 81 years old. No correlation was apparent between the specified SARS-CoV-2 specific IgG and IgM immunoglobulin levels of the positive group, their sex, or age. Raman spectroscopic measurements were performed at 785nm, in liquid serum, thawed from frozen, and spectra were pre-processed to remove the contribution of water, normalising to the water content. Principal components analysis of the spectral dataset over the range 400-1800 cm^{-1} provided no clear indication of a difference between normal serum and SARS-CoV-2 positive serum. A selection of 5 of the samples, which were available in sufficient volume, were fractionated by centrifugal filtration, and the 100kDa, 50kDa, 30kDa, and 10kDa concentrates similarly analysed by Raman spectroscopy. Partial least squares regression analysis revealed a negative correlation between the spectral profile of the 30kDa fractions and SARS-CoV-2 specific IgG antibody levels, potentially indicating an association with depleted glutathione levels. The study supports a potential role of Raman screening of blood serum for monitoring of SARS-CoV2 infection, but also in longitudinal studies of disease progression, long term effects, and therapeutic interventions.

[1] Glassman I, Le N, Mirhosseini M, Alcantara CA, Asif A, Goulding A, et al. The Role of Glutathione in Prevention of COVID-19 Immunothrombosis: A Review. Front Biosci (Landmark Ed)
[2] Kumar P, Osahon O, Vides DB, Hanania N, Minard CG, Sekhar R V. Severe glutathione deficiency, oxidative stress and oxidant damage in adults hospitalized with covid-19: Implications for glynac (glycine and n-acetylcysteine) supplementation. Antioxidants. 2022;11.

Keywords: Raman Spectrocopy, COVID-19, Human Serum, Glutathione

Nanoparticles of the $CaTiO_3$ system: Synthesis, characterization and evaluation of their ability to degrade emerging contaminants

Lizet Cerón[1,2], Carol Aguilar[1,2], Jesús Evelio Diosa[1,2], Edgar Mosquera[1,2]
[1]Department of Physics, Universidad del Valle, Group of Phase Transitions and Functional Materials, Faculty of Natural and Exact Sciences, Universidad del Valle, Santiago de Cali, Colombia.
[2]Center of Excellence in New Materials (CENM), Universidad del Valle, Santiago de Cali, Colombia.

Emerging pollutants are compounds of various origin and chemical nature, whose presence in the environment is not considered significant in terms of distribution and concentration, so they go unnoticed. There is currently a growing interest in emerging pollutants (ECs), since they cause environmental problems and health risks. These compounds are disseminated in the environment and have been detected in water supply sources, groundwater, and even in drinking water. They are compounds of which relatively little is known, in terms of their presence, impact and treatment; in most cases they are unregulated contaminants, which may be candidates for future regulation, depending on research on their potential health effects and monitoring data regarding their incidence; therefore, they are amenable to investigation. Major ECs include pesticides, pharmaceuticals, illicit drugs, "lifestyle" compounds, personal grooming, and others [1], [2]
In the present research work, the photocatalytic capacity of nanoparticles of the $CaTiO_3$ system was evaluated, specifically methyl orange (NM) and levofloxacin (LVF), considered emerging contaminants, non-biodegradable when dissolved in water. Ceramic powders were obtained using the Polymeric Precursor (Pechini) method. The nanoparticles of the oxide of interest obtained were characterized using ultraviolet spectroscopy with diffuse reflectance (UV-vis DRS), to know the electronic transitions and determine the value of the forbidden band of energy; IR spectroscopy, to determine the functional groups present in the samples; as well as X-ray diffraction (XRD), to determine the crystalline phases existing in the solid, and scanning electron microscopy (SEM) to observe the size, morphology and degree of agglomeration of the particles. The powders obtained were studied for their ability to act as a photocatalyzing agent for a glyphosate-based agrochemical (GBH) dissolved in water. For this purpose, UV-visible spectroscopy was used considering the variation of the intensity of the characteristic band of greater absorption, which was correlated with the change in the concentration of the agrochemical in the solution (previously establishing an absorption calibration curve - contaminant concentration). For the study, different pH conditions and incidence of UV radiation on the system were considered.

[1] M. J. Gil, A. M. Soto, J. I. Usma, and O. D. Gutiérrez, “Contaminantes emergentes en aguas, efectos y posibles tratamientos,” Prod. + Limpia, vol. 7, no. 2, pp. 52–73, 2012, Accessed: May 26, 2023. [Online]. Available: http://www.scielo.org.co/scielo.php?script=sci_arttext&pid=S1909-04552012000200005&lng=en&nrm=iso&tlng=es.
[2] D. Jacobo-marín, “Contaminantes emergentes en el agua : Regulación en México , principio precautorio y perspectiva comparada,” vol. 15, pp. 51–76, 2021, doi: 10.5354/0719-4633.2021.57414.

Acknowledgements: This work was supported by projects SGR BPIN 2021000100424, 2020000100377 and postgraduate in physical sciences of universidad del Valle.

Keywords: Polymeric precursor method, photocatalysis, optical properties, water treatment, emergent contaminants.

Development of novel capsule-based delivery systems targeting agri-food applications

Vasco D.F. Martins[1,2], Miguel A. Cerqueira[2], Lorenzo M. Pastrana[2], José A. Teixeira[1] and Pablo Fucinõs[2]

[1] *Centre of Biological Engineering, University of Minho, Campus de Gualtar, 4710-057, Braga, Portugal.*
[2] *International Iberian Nanotechnology Laboratory, Av. Mestre José Veiga, 4715-330, Braga, Portugal.*
vasco.martins@inl.int

Recent developments with encapsulation of active compounds have helped to overcome challenging problems in agrifood sector, from phage-based therapeutics for pathogenic resistant strains to application of essential oils or pesticides [1]. In this work, two new delivery systems were developed using electrospraying technique (Figure 1). These systems were optimized using different biopolymers, namely, Fibruline® and shellac gum with hydroxypropyl methylcellulose (HPMC) or by the addition of surfactants to improve sprayability. From the 250 trials performed, two optimized formulations were selected: 20% (w/v) shellac gum, 15% (w/v) Fibruline and 2% (w/v) Tween 80 (SFT); and 3% (w/v) HPMC, 3% (w/v) shellac gum and 2% (w/v) Fibruline (HSF). Using HSF it was possible to decrease the voltage (from 22 to 16 kV) which can be fundamental for the stabilization of the bioactive compound to be encapsulated; and the distance (from 26 to 17 cm) that allows to increase the yield of the process. Concerning particles' morphology, those HSF showed greater sphericity, smoother surface and a narrower size distribution. The particles obtained with SFT and HSF presented a mean diameter of 997±573 nm and 676±260 nm, respectively. Regarding solution viscosity, HSF presented a higher value that can explain improved physical properties of the dispersion and, therefore, improved sprayability and particles' morphology. Concerning surface tension, SFT and HSF presented similar values. In terms of conductivity, SFT showed to be much more conductive, which justifies the presence of very small particles with multiple morphologies attained to the bigger ones. In conclusion, we were able to develop and produce new delivery systems with great potential for stabilising and improving bioavailability of bioactive compounds of interest.

[1] G.L. Zabot, F.S. Rodrigues, L.P. Ody, M.V. Tres, E. Herrera, H. Palacin, J.S. Córdoba-Ramos, I. Best and L. Olivera-Montenegro, Encapsulation of Bioactive Compounds for Food and Agricultural Applications. Polymers. 14, 4194 (2022).

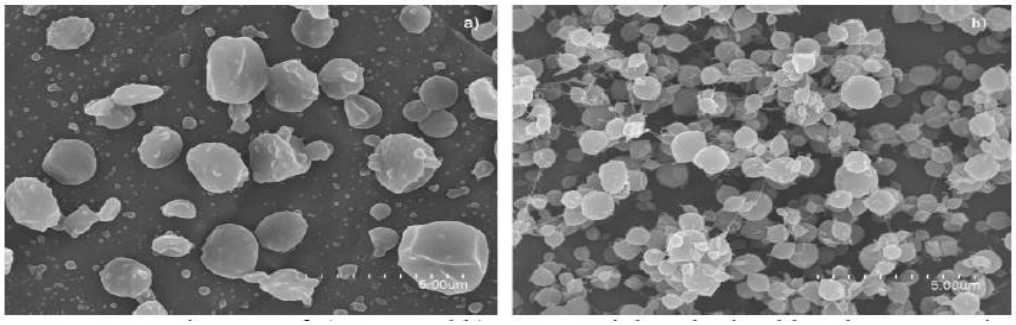

Figure 1. SEM images of a) SFT and b) HSF particles obtained by electrospraying.

Acknowledgements: This study was supported by the Portuguese Foundation for Science and Technology(FCT) under the scope of the strategic funding of UIDB/04469/2020 unit, and by LABBELS – Associate Laboratory in Biotechnology, Bioengineering and Microelectromechanical Systems, LA/P/0029/2020, and the fellowship SFRH/BD/148504/2019. This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 778388.

Keywords: Delivery systems; Encapsulation; Agrifood Technology; Biopolymers.

Nanotechnologies and regulation: possibility of a regularoty interface between technical norms and the Law as protection for researchers/producers and society

Patricia Santos Martins[1]
1 Universidade do Vale do Rio dos Sinos,Grupo de Pesquisa JUSNANO, São Leopoldo/RS, Brazil; patricia.mart@hotmail.com

The theme of this research project is "Nanotechnologies and regulation: the possibility of a regulatory interface between technical standards and the Law as protection for researchers/producers" and studies self-regulation and the possibility of protecting rights that are already assured, such as the right to information, health, life, and the environment[1]. And also, it is circumscribed in the field of scope and performance of the ISO standards adopted by Brazil through ABNT, to identify how they contribute to the protection of these legal assets, in order to observe possible regulatory interfaces between the technical standardization system and the legal order. It seeks to describe what are the definitions, characteristics and development of nanotechnologies, and their objectives in their diversity of techniques and applications. In addition, the development from the normative perspective, the existence or not of nanospecific norms in force in Brazil, and what would be the existing principles in the legal system for the protection of the already protected rights and the possible interrelationships with principles and constant guidelines of technical norms[2] – with the aim of making up for the lack of nanospecific regulatory frameworks. Consequently, it seeks to analyze the concept and effectiveness of self-regulations systems[3], legal pluralism and the technical normalization system to identify the social perceptions regarding the possible interfaces. The chosen methodology is the historical and comparative functionalist, which seeks to establish analogies between the various forms of cultural and social organization and, for the human sciences, seeks to emphasize the relationships between different components of a culture or society. With the compilation of data, connections will be developed between the theoretical possibilities and the answers found throughout the proposed course, to highlight the real chances that self-regulatory systems serve as alternatives for the safe and informative development of disruptive technologies not yet regulated by State legislative monopoly.

[1] MARTINS, Patricia Santos. As Nanotecnologias e as Normas ISO: estruturando a governança regulatória por normas técnicas. URI: http://www.repositorio.jesuita.org.br/handle/UNISINOS/10094.
[2]FRYDMAN, Benoit. Breve manual práctico de derecho global. Traducción de Bernardo Carvajal Sánchez. Bogotá: Universidad Externado de Colombia, 2018.
[3] TEUBNER, Gunther. Fragmentos Constitucionais: Constitucionalismo social na globalização. Coordenação Ricardo Campos. ISBN: 9788553617531. São Paulo: 2020.

Acknowledgements: The author would like to thank Prof. Doctor Wilson Engelmann for his support and guidance throughout the research.

Keywords: Law and regulation, Regulatory Public Law, Nanotecnologies and Human Rights.

Micro and nano encapsulation systems of resveratrol and melanoidins in the context of circular economy

Pedro M. Silva[1,2], Mafalda Neto[3], Lorenzo Pastrana[3], Manuel A. Coimbra[3], Catarina Gonçalves[3], António A. Vicente[1], Miguel A. Cerqueira[2]

1 Centre of Biological Engineering, University of Minho, 4710-057 Braga, Portugal
2 International Iberian Nanotechnology Laboratory, Av. Mestre José Veiga s/n, 4715-330 Braga, Portugal
3 LAQV-REQUIMTE, University of Aveiro, 3810-193 Aveiro, Portugal
miguel.cerqueira@inl.int

Bioactives that can be recovered from by-products of food industries can have interesting applications in other industries, a concept referred to as circular economy. These bioactives can have several bioactivities, such as antimicrobial and antioxidant, that can be useful for several industries, namely food, pharmaceutic, and agricultural industries. As such the aim of this work is the development of versatile micro-nanoencapsulation systems using electrohydrodynamic processing and emulsification techniques, using industrial by-products, namely resveratrol and coffee melanoidins. At first, it was necessary to develop micro-and nanostructures that could encapsulate the desired bioactives. To do so two techniques were used, electrohydrodynamic processing (EHDP) and high energy emulsification. Both particles and fibres were developed using EHDP from hydroxypropyl methylcellulose of different molecular weights, as different micro-and nanostructures morphologies can display different properties (e.g., bioactive incorporation, release kinetics and protection). These systems were optimized using a Design of Experiments methodology, which allowed to determine the influence of the several processing parameters (polymer concentration, flow rate, voltage, and tip-to-collector distance) on fibre or particle diameter, PDI, particle aspect ratio or fibre break percentage of the produced structures. After, melanoidins (loading of 2.5 mg/mL solution) and resveratrol (loading of 0.75 mg/mL solution) were successfully loaded, and all micro-and nanostructures (or polymer solutions) were characterized regarding their rheological, thermal, chemical, and morphological properties. Melanoidin- and resveratrol-loaded spherical microparticles and continuous thin nanofibers were produced. High-speed homogenization and ultra-sonication were used for the development of resveratrol-loaded emulsions. Oil-in-water emulsions were produced with sunflower oil and sodium octenyl succinic anhydride modified starch (OSA-MS) in a 5:95 ratio. Resveratrol was dispersed in the oil phase and encapsulated at a loading of 7.5 mg/mL of emulsion. Obtained emulsions were small (210 nm) with a low PDI (0.266), presenting a Zeta potential of -62.5 mV. They were stable for around 90 days when stored at 4 and 23 °C. Foreseeing possible applications in the agricultural industry, namely as an antimicrobial or antioxidant agent in plants (e.g., applied in crops or even in fruit sold in supermarkets), the emulsions and the HPMC microparticles were assessed regarding their cytotoxicity and their antioxidant activity (measured through ROS production), before and after an in vitro digestion. All tested samples had a high cell viability, indicating their biocompatibility to be used on the surface of plants or fruits that are suitable for human consumption. Encapsulated samples displayed better results compared to unencapsulated samples regarding antioxidant activity, highlighting resveratrol's improved performance due to encapsulation.
In conclusion, versatile, food-grade micro- and nanostructures were successfully developed with potential to encapsulate both hydrophilic and hydrophobic bioactives that could potentially be used on the surface of plants, crops and fruits fit for human consumption and that can provide antioxidant activity.

Keywords: electrohydrodynamic processing; resveratrol, HPMC, starch

Synthesis of zinc and iron oxides nanocomposites for water remediation: ammonium removal studies

María Belén Perez Adassus[1], Carla Vanesa Spetter[1,3] and Verónica Lassalle[1,2]
1 Departament of Chemistry, University National of South (UNS), Av. Alem 1253, Bahía Blanca, B8000, Argentina
2 Institute of Chemistry of South (INQUISUR),CONICET/UNS, Av. Alem 1253, Bahía Blanca, B8000, Argentina
3 Institute Argentinian of Oceanography (IADO), CONICET/UNS, Camino La Carrindanga Km 7.5, Edificio E1, FWB, Bahía Blanca, Buenos Aires B8000, Argentina. belen.adassus@uns.edu.ar

Ammonium (NH_4^+) is an inorganic cation present in nature as part of the biogeochemical cycle of nitrogen. It is a source of nutrients for microorganisms living in aquatic environments. In the last decades, the presence of NH_4^+ in water has increased due to the extensive use of agricultural fertilizers, the sewage discharges without any decontamination treatment, and industrial activity in general [1]. The use of different organic dyes in textile industries and its final deposition, has become a great problem for environment. These organic compounds can change the coloration of water bodies and therefore inhibit the correct penetration of sun light, giving place to water quality deterioration by modifying the CO_2 absorption for photosynthesis process. These compounds are toxic by composition too, and can bioaccumulate on aquatic species tissues. Therefore, the development of efficient water remediation technologies is crucial to address the challenge of removing NH_4^+ and dyes from water sources. Zinc oxide nanoparticles (ZnO NPs) are particularly interesting because of their photocatalytic and antibacterial potential for use in diverse application fields. Despite the good efficiency of this material, there are some limitations related to their separation from the reaction medium. Conventional separation methods such as filtration and centrifugation are expensive, tedious, generate extra residues, and are unviable to scale up. In this concern, magnetic separation seems to be an alternative to mitigate these drawbacks. Iron oxides superparamagnetic nanoparticles, like magnetite (Fe_3O_4) and maghemite have an excellent adsorption capacity and can be easily and quickly separated from the reaction medium by applying an external magnetic field generated by a simple magnet. When iron oxides combine with zinc oxide nanoparticles a synergy of their properties occurr improving their performance for water remediation applications [2]. In this work, two nanomaterials (MCZ1 and MCZ2), based on zinc oxide nanoparticles and iron oxide nanoparticles were synthesized. For MCZ1, ZnO and Fe_3O_4 nanoparticles were contacted in an ultrasonic bath for 2 hours, at 160W and 40 Hz. The nanomaterial MCZ2 was prepared by seed method, to this, an amount of previously synthesized Fe_3O_4 nanoparticles were dispersed in water with zinc salts and NaOH solution (5M) dropwise added from a burette. The nanomaterials obtained were characterized by different techniques. From DRX analysis, the crystalline pattern of ZnO and Fe_3O_4 was indexed to both nanomaterials. FTIR revealed Zn-O vibration mode (~ 500 cm^{-1}) and Fe-O stretching mode, corresponding to the octahedral and tetrahedral sites of cubic spinel magnetite at 570 cm^{-1} and 390 cm^{-1}, respectively. The application of these materials to assess the ammonium elimination from water bodies by adsorption was investigated. The experimental data demonstrated efficiency of 0.99 mg of NH_4^+ adsorbed per gram of nanomaterial MCZ1. To explore dual activity of these composites, photodegradation of metilene blue as a model dye was explored by using a 15W, UV lamp. The results show a degradation of 97% of dye by the nanomaterial MCZ2 at 120 minutes.

[1] Q. Yin, L. et al., Chemosp. 287, 132294 (2022).
[2] I. E. Medina-Ramírez et al., Ceram. Int. 46, 7 (2020).

Acknowledgements: This work was supported by CONICET, UNS, IADO and INQUISUR. The authors would like to thank to FAPESP and CNPEM for the schoolarship to assist SPSAS NanoAgri&Enviro.

Keywords: Zinc and Iron Oxide nanocomposites; Water Remedation; Ammonium removal; Photodegradation.

The Emergence of Nanophytovirology: A Promising Paradigm for Plant Virus Disease Management

Raja muthuramalingam Thangavelu and Washington Luis da Silva
Department of Plant pathology and Ecology, Connecticut Agricultural Experiment Station, New Haven, 06511, Connecticut, United States of America.
Email raja.muthuramalingam@ct.gov

Nanophytovirology has emerged as an advanced and promising approach in the field of plant viral disease control. This interdisciplinary field capitalizes on the distinctive physiochemical properties of nanoparticles (NPs) to engage with viruses, their vectors, and host plants in targeted and advantageous ways. By integrating principles from nanotechnology and virology, our team aims to pioneer the development of innovative nanoscale tools for the prevention and treatment of plant diseases. The objective of my presentation is to provide an encompassing overview of the current state of nanophytovirology, encompassing its applications, limitations, and future directions. The convergence of nanomaterials and plant virology offers unparalleled prospects for combating devastating plant pathogens. Nanophytovirology encompasses a range of strategies, including the creation of nanocarriers for precise delivery of antiviral agents and the utilization of nanosensors for real-time monitoring of plant viral diseases. These advancements facilitate accurate and efficient interventions in disease management.While nanophytovirology continues to evolve, it presents exciting opportunities for future growth and impact. Sustained research and development efforts in this field will pave the way for the advancement of innovative nanoscale tools, enabling sustainable and effective control of plant viral diseases.

[1] Tahir et al., Nanotechnology and plant viruses: an emerging disease management approach for resistant pathogens, ACS Nano 2021, 15, 4, 6030–6037.
[2] Raja muthuramalingam, Ultra-sensitive nano-gold labelled, duplex lateral flow assay for early detection of sugarcane mosaic virus, Scientific Reports, 2022, 12, 4144.
[3] Washington et al., Nano enabled delivery of RNA molecules for prolonged antiviral protection in crop plants: A review, ACS Appl.Nano Mater. 2021, 4,12.

Acknowledgements: This work was supported by National Institute of Food and Agrciutlure-(SID23107), USA.

Keywords: Plant viral diseases, nanotechnology, disease management, sustainable agriculture

Effects of different biogenic silver nanoparticles on the routine metabolism of *Astyanax ribeirae*

Renata Antunes Portis[1], Luiz Gustavo Ribeiro[2] and Edison Barbieri[1]
[1] *Instituto de pesca, Secretaria de Agricultura e Abastecimento, de São Paulo, (SAASP) , 11990-000, Cananéia, Brazil;*
[2] *Instituto Butantan, Development and Innovation Laboratory, 05503-900, São Paulo, Brazil.*
edisonbarbieri@yahoo.com.br

In this study, the toxic effects of different types of biogenically sourced silver nanoparticles (AgNPs) on the metabolism of *Astyanax ribeirae*, also known as lambari, were investigated. AgNPs are widely used in aquaculture for disease control and water treatment, necessitating the assessment of their potential negative impacts on aquatic organisms [1]. Exposures of lambari to different types of AgNPs (sugarcane bagasse, coated, and mycogenic) were conducted for 24 hours, with routine metabolism indicators, such as oxygen consumption and ammonia excretion, measured as toxicity indicators [2]. The results indicated that lambari exposed to sugarcane bagasse AgNPs exhibited a significant reduction in oxygen consumption at concentrations of 100 µg, while ammonia excretion increased at concentrations of 1000 µg. These effects demonstrated a dose-dependent relationship, indicating that higher concentrations of AgNPs led to more pronounced metabolic changes. In the case of coated AgNPs, a gradual decrease in oxygen consumption and a reduction in ammonia excretion were observed at concentrations of 100 µg. However, at higher concentrations (100 and 500 µg), an increase was observed compared to the control group. With mycogenic AgNPs, both oxygen consumption and ammonia excretion increased gradually with increasing concentrations, also following a dose-dependent relationship. The observed metabolic responses in lambari exposed to different AgNPs are highly significant and contribute to a better understanding of the potential toxic effects of these nanomaterials. It is important to note that despite all AgNPs used in this study being of biogenic origin, each one exhibited distinct responses, emphasizing the importance of conducting toxicity tests regardless of the biosynthesis form of AgNPs. The findings highlight the need for careful evaluation of the effects of AgNPs in the aquatic environment, particularly in economically and environmentally important species like lambari. This information is crucial for ensuring the safety and responsible use of these nanomaterials in aquaculture and other water and environmental-related fields.

[1] A. Baranwal, A. Srivastava, P. Kumar, V. Bajpai, P. Maurya, P. Chandra. Prospects of Nanostructure Materials and Their Composites as Antimicrobial Agents. Front. Microbiol. 9, 422 (2018).
[2] L.G. Ribeiro, G.S.C Roque, R. Conrado and A. O. De Souza. Antifungal Activity of Mycogenic Silver Nanoparticles on Clinical Yeasts and Phytopathogens**.** Antibiotics. 12, 91 (2023).

Acknowledgements: This work was supported by CAPES; CNPq and FAPESP.

Keywords: Silver nanoparticles, aquaculture, ecotoxicology

Absorption and localization of lignin nanoparticles in Solanum lycopersicum leaves

Faleiro, Rodrigo[1], Fraceto, Leonardo[2], Barbosa, Anderson[2], Tesmer, Magda[3] and Mayer, Juliana[1].
1 State University of Campinas, Department of Plant Biology, Campinas, Brazil.; 2 State University of São Paulo, Department of Environmental Engineering, Sorocaba, Brazil. 3 University of São Paulo, Department of Biological Sciences, Piracicaba, Brazil.
rodrigofaleiroflorestal@gmail.com

The concern about population growth has raised several questions regarding the production efficiency in different globally planted agricultural crops. The need for increased production on smaller temporal and spatial scales has sparked the demand for the development of new technologies. Among them, the use of nanoparticles (NPs) in agriculture has proven to be an effective and cost-efficient option, transporting herbicides or growth regulators (GRs) to the desired location, promoting sustained release and enhanced efficacy of the target molecule. Therefore, determining the absorption mode and the time at which these nanoparticles can be absorbed, as well as the compartmentalization site, aids in understanding the processes involved in the release of the target molecule. Given this scenario, our study aims to understand the mechanisms of absorption of lignin nanoparticles (LNPs) and the cellular localization of these particles in leaf samples of Solanum lycopersicum hybrid "Sweet Grape". For this purpose, the LNPs were marked with Liss Rhod PE and sprayed onto Tomato plants at a concentration of 100 ppm of LNPs. Collections were made at 0, 1, 2, and 9 hours after application, with five replicates per collection. The samples were subjected to standard scientific methodology for confocal microscopy analysis, which was performed using a Zeiss LSM780-NLO upright confocal microscope with excitation at 552 nm and emission ranging from 572 to 607 nm at INFABiC/Unicamp. As results, we identified that LNPs can be absorbed primarily through stomata, but they can also penetrate the cuticle and the walls of epidermal cells. Starting from 1 hour after application, LNPs were observed on the leaf surface and within the parenchymal cells of the mesophyll. After 2 hours of application, they were already found within the leaf parenchymal cells, and after 9 hours of application, they are present in most of the mesophyll cells and in the cells of the sheath near the vascular bundles, where they can be transported to other organs. Therefore, LNPs exhibit both polar transport (entry through stomata, hydrophilic) and nonpolar transport (entry through pores in the cuticle, hydrophobic), demonstrating excellent absorption within a short period. These results indicate that lignin nanoparticles can be effectively used for delivering different molecules into plant tissues with different uses.

Acknowledgements: The authors would like to thanks CNPq and FAPESP for the scholarship and financial suport.
Keywords: crop science, nanotecnology, plant tissue.

AI-assisted robotic manipulation of plant cells

Sabrina Gennis[1] and Kaare H. Jensen[2]
[1]*Technical University of Denmark, Department of Physics, Kongens Lyngby, Denmark*
sabge@dtu.dk

There has been a growing demand for sustainable and renewable sources of energy, with biofuel being one of them. The production of biofuel relies on the sugar of harvested plants. However, using whole crops takes up agricultural space which could otherwise be used to meet the increasing demand in food supply. An improved method to obtain the sugar for biofuel production could be to directly and sustainably extract sugar from plants. Sugar as well as other molecules, which might be of interest as pharmaceuticals, are often localized in specific cells in the plant. Already, an autonomous extraction of metabolite-rich surface cells from leaves has successfully been obtained[1]. The sugarrich phloem however is located deeper within the tissue of plants and a high quantity, autonomous extraction has yet to be achieved. The limit in quantity is mostly due to the plant's defense response to wounding which leads to a closing of the phloem flow. To overcome this response, I propose to overstimulate the plant by using methods such as continuous touch, electroshock, drastic temperature changes, laser exposure, and more. In the first step, I built a high-resolution, multifunctional robot. The next step was to design different probes to manipulate plant leaves and measure their defense responses. The robot will be used to mount the various probes and manipulate the plants autonomously. Eventually, it will be guided by computer vision using machine learning algorithms to find its target regions. If the defense mechanisms can successfully be overcome, and the phloem successfully targeted, then sugar-rich phloem sap can be extracted and potentially be used in biofuel production. The results will lead towards making biofuel production more sustainable.

[1] H. Bae, M. Paludan, J. Knoblauch, K.H. Jensen, Neural networks and robotic microneedles enable autonomous extraction of plant metabolites, Plant Physiology, (2021), 186, 1435-1441.

Keywords: plant defense, robotics, renewable energy, biofuel

Evaluation of PVA hydrogels for the entrapment of biogenic Ag-NPs in water disinfection treatment

Iancilevich, Santiago A.[1]; Herold, I. E.[2]; Bacigalupe, A.[2]; Escobar, M.[2]; Perullini, A. M.[3]; Spagnoletti, F.[1]; Giacometti, R.[1*]

1 INBA-CONICET, Facultad de Agronomía, UBA, Avda. San Martín 4453, C1417DSE, Buenos Aires, Argentina.

2 Instituto Nacional de Tecnología Industrial, Av. General Paz 5445, B1650WAB, San Martín, Buenos Aires, Argentina.

3 CONICET-Universidad de Buenos Aires. INQUIMAE, Intendente Güiraldes 2160, C1428EGA, Buenos Aires, Argentina.

siancilevcih@agro.uba.ar

The development of new water treatment techniques is motivated by the global scarcity of quality drinking water, which jeopardizes public health, social dignity, and economic development [1]. The main goal of this study was to develop a modified material that combines biocidal silver nanoparticles (Ag-NPs) with a polymeric hydrogel matrix that can disinfect water for human consumption. Biogenic Ag-NPs have been successfully synthesized and characterized, and their biocidal activity has been evaluated in microbial cultures. Currently, it is of interest to establish manufacturing conditions for PVA hydrogels that meet suitable properties for safe use in water treatment, which is crucial for the development of hydrogels with a robust structure that can maintain their conformation and effectively retain Ag-NPs within their matrix. Additionally, hydrogels should exhibit an excellent swelling capacity to facilitate water diffusion into their interior and promote contact between microorganisms and biocidal NPs. PVA hydrogels were prepared at different concentrations (5, 7.5, 10, and 12%), with 4 freeze-thaw cycles (2, 4, 6, and 8 cycles) and 2 freeze-thaw durations (16-1 h and 23-1 h). The structure of the hydrogels was analyzed by rheology, which enabled the study of the evolution of the elastic (G') and viscous (G'') moduli under varying strain levels [2]. Water retention (WR%) and swelling (H%) were evaluated using gravimetric analysis [3]. The WR% was studied by drying the samples at 40 °C for 4 h and weighing every 15 min. H% was studied by hydrating the dry samples in distilled water at 25 °C for 3 h and weighing every 10 min. PVA hydrogel samples were successfully synthesized. Rheological analysis provided information on the viscoelastic behavior of the hydrogels. A higher concentration of PVA, along with an increased number of cycles, resulted in higher elastic modulus values, indicating an enhancement in the hydrogel structure. Furthermore, it was consistently observed that hydrogels with a concentration of 7.5%, subjected to 2 cycles, and frozen for 16 h exhibited a higher WR% when dried. In terms of H%, hydrogels with a concentration of 5%, a freezing duration of 23 h, and 2 freeze-thaw cycles exhibited a higher swelling capacity. The characterization techniques used in this study allowed us to select the optimal synthesis conditions for the hydrogels: a low concentration of PVA and a reduced number of freeze-thaw cycles. The differences observed in water retention and swelling can be attributed to variations in the size and distribution of pores between the hydrogels fabricated under different conditions. Based on these results, the samples to be used in subsequent stages of this study can be established to achieve secure entrapment of Ag-NPs and perform water sample disinfection. In a next step, these results can serve as a reference for the development of hydrogels based on PVA, combined with starch, sodium alginate, and chitosan. This study will include other characterization techniques, such as SEM, re-swelling, and diffusion tests, for these materials to further enhance our understanding of these systems.

[1] Connor, R., & Koncagül, E. (2015). Informe de las Naciones Unidas sobre los recursos hídricos en el mundo 2015: Agua para un mundo sostenible. Resumen ejecutivo.

Green electrospinning of organic-inorganic hybrid system

Soraia A.R. Coelho[1], Jula Kniep[2], Nathalie Barroca[3], M.H.V. Fernandes[1], J.C. Almeida[1]
[1]University of Aveiro, Department of Materials and Ceramic Engineering, CICECO - Aveiro Institute of Materials, 3810-193, Aveiro, Portugal; [2]University of Applied Sciences, Faculty 5-Nature and Engineering, Neustadtswall 30, 28199 Bremen, Germany; [3]University of Aveiro, Mechanical Engineering Department, Center for Mechanical Technology & Automation (TEMA), 3810-193 Aveiro, Portugal.
soraia.coelho@ua.pt

Organic-inorganic hybrid materials are a potential alternative of materials with superior features and have been applied in many fields. Particularly, poly(ε-caprolactone) (PCL), a synthetic biodegradable polymer, and bioactive glass (BG), an inorganic biomaterial, have shown promising results in tissue engineering. Their combination at the nanoscale allows the integration of multiple properties, such as mechanical strength, hydrophilicity, biocompatibility, as well as controlled degradation behaviour. Sol-gel is a viable route to combine both. To mimic the natural biological structure of extracellular matrix, the polymer solution can be electrospun into nanofibers meshes. Generally, toxic solvents are used to dissolve the polymer, but recently the concept of "green electrospinning" has been reported with promising results, based on benign solvents [1]. Aim: to develop and characterize multicomponent nanofibrous meshes, by electrospinning, using a polymeric matrix combined with boron and calcium silicate glass, formed via in situ sol-gel, and based on a green fabrication route. PCL and PCL/SiO2-B2O3-CaO compositions were prepared with different green solvent systems and characterized [2]. ATR-FTIR spectroscopy confirmed intermolecular hydrogen-bonding interactions between the carbonyls of PCL and the hydroxyls (Si-OH) of silica networks. Also, the linkage between boron and silica was confirmed by solid state ^{11}B NMR technique, where peaks assigned to the trigonal BO_3 and tetrahedral BO_4 groups were found. Thermal analysis revealed a change in the crystallinity of PCL with the incorporation of inorganic domain, while SEM/EDS showed a uniform distribution of Ca and Si elements in the fibers. Concluding, green PCL/boron and calcium-containing silicate compositions were suitable for electrospinning into fibrous meshes.

[1] L. Liverani, J. Lacina, J.A. Roether, E. Boccardi, M.S. Killian, P. Schmuki, D.W. Schubert, A.R. Boccaccini, Incorporation of bioactive glass nanoparticles in electrospun PCL/chitosan fibers by using benign solvents, Bioact Mater. 3 (2018) 55–63.
[2] S.A.R. Coelho, J. Kniep, N. Barroca, J.C. Almeida, M.H.V. Fernandes, Nanofibrous hybrid scaffolds based on PCL-borosilicate system by a green sol-gel process, Mater Today Chem. 29 (2023).

Acknowledgements: This work was developed within the scope of the project CICECO-Aveiro Institute of Materials, UIDB/50011/2020, UIDP/50011/2020 & LA/P/0006/2020, financed by national funds through the FCT/MCTES (PIDDAC). The NMR spectrometers are part of the National NMR Network (PTNMR) and are partially supported by Infrastructure Project Nº 022161 (co-financed by FEDER through COMPETE 2020, POCI and PORL and FCT through PIDDAC). This work is also financed by national funds through FCT-Fundação para a Ciência e Tecnologia, I.P., within the scope of the doctoral grant 2021.05864.BD.

Keywords: nanofibers, green solvents, poly(ε-caprolactone), borosilicate

Effect of ion exchange and calcination temperature on the magnetic properties of sodium titanate nanotubes

Tainara Gomes De Oliveira[1], Yuset Guerra[2], Ramón Raudel Peña Garcia[3], Suziete Batista S. Gusmão[2], Suzana Araújo-Barbosa[4], Anderson O. Lobo[1], Edson C. Silva-Filho[1], And Bartolomeu Cruz Viana Neto[1,2]

[1] Federal University of Piauí, Department of Materials Science and Engineering, 64049-550, Teresina, Brazil; [2] Federal University of Piauí, Department of Physics, 64049-550, Teresina, Brazil; [3] Federal Rural University of Pernambuco, Academic Unit Cabo de Santo Agostinho, 54518-430, Cabo de Santo Agostinho, Brazil; [4] Federal University of Rio Grande do Norte, Department of Physics, 59078-970, Natal, Brazil.
Email: tainaragomes96@gmail.com

Sodium Titanate nanotubes, NaTiNT, are structures with nanotubular morphology, hollow cavity, and layered walls. They consist of hydroxyls, OH^-, in the external region and sodium ions, Na^+, in its internal region. NaTiNTs are synthesized by the alkaline hydrothermal method, with TiO_2 as a precursor and sodium hydroxide as an alkaline base. These nanostructures have favorable structural and morphological properties to evaluate their effect on dye-sensitized solar cells, proton conduction, photocatalysis, and spintronic devices, among other applications, due to the high specific surface area, high pore volume, and ion exchange capacity [1,4]. In this work, NaTiNTs were synthesized by the hydrothermal method and submitted to the ion exchange reaction process with Fe^{3+}, Co^{2+}, and Ni^{2+} ions to evaluate their magnetic behavior when subjected to the action of an external magnetic field. In addition, the samples obtained were calcined in contact with atmospheric air at 400 °C and 800 °C. All the material obtained was characterized by Ray Diffraction - X, Raman Spectroscopy, UV-Vis in Diffuse Reflectance, and Magnetometry of Vibrant Sample. The samples of Titanate nanotubes exchanged ionically, when calcined at 400 °C, suffered a breakdown of the nanotubular structure, and 800 °C structures were transformed into phases related to anatase and rutile TiO_2, effect perceived by XRD and Raman Spectroscopy. Studies of Diffuse Reflectance showed that samples with Fe^{3+}, Ni^{2+}, and Co^{2+} promoted a decrease in the energy gap when the samples were calcined at 400 °C because, at this temperature, there is a greater number of defects in the structure, such as oxygen vacancies, which can be measured by calculating the Urbach Energy. By the magnetometry of the vibrating sample, it was possible to observe ferromagnetic behavior in all samples in smaller external magnetic fields. This behavior is caused by interactions between the intercalated ions in the nanotube walls, by oxygen defects that arise with calcination, and by the transition from Ti^{4+} to Ti^{3+} in some sites of the nanotubular structure. Given these results, these materials can be promising spintronic materials and can be used as diluted magnetic semiconductors [2-6].

[1] Ali, T.; Ahmed, A.; Siddique, M. N.; Alam, U.; Muneer, M.; Tripathi, P. Optik, 223, 165340, 2020.
[2] Gusmão, S. B. S.; et al. Journal of Physics and Chemistry of Solids, 145, 2020.
[3] Li, R.; Zhang, F.; Zhang, J.; Dong, H. International Journal of Hydrogen Energy, v. 47, p. 5260-5268, 2022.
[4] Oliveira, T. G.; et al. Journal of Materials Research, 1-17, 2023.
[5] Saliu, O. D.; Mamo, M.; Ndungu, P.; Ramontja, J. Journal of Energy Storage, v. 49, 104155, 2022.
[6] Silva, J. P.; et al. Journal of Alloys and Compounds, v. 867, 159025, 2021.

Acknowledgements: This work was supported by CAPES. The authors would like to thank UFPI, PPGCEM, LIMAV, and FISMAT.

Keywords: titanate nanotubes, ferromagnetism, defects.

Nanotoxicity Assessment of Graphene oxide – Gold Nanohybrid on *Daphnia Magna*

Taiwo Hassan Akere [1,2,*], Aline M. Z. de Medeiros[3,4], Diego Stéfani T. Martinez[3,4], Bashiru Ibrahim[1,2], Hanene Ali-Boucetta[2] and Eugenia Valsami-Jone[1,*]

[1] *School of Geography, Earth and Environmental Science, College of Life and Environmental Sciences, University of Birmingham, Birmingham B15 2TT, UK*

[2] *Nanomedicine, Drug Delivery & Nanotoxicology (NDDN) Laboratory, School of Pharmacy, College of Medical and Dental Sciences, University of Birmingham, Birmingham B15 2TT, UK*

[3] *Brazilian Nanotechnology National Laboratory (LNNano), Brazilian Centre for Research in Energy and Materials (CNPEM), Campinas 13083-100, SP, Brazil*

[4] *Centre of Nuclear Energy in Agriculture (CENA), University of São Paulo (USP), Piracicaba 13416-000, SP, Brazil*

t.akere@bham.ac.uk; e.valsamijones@bham.ac.uk

Contemporary research in nanomaterials is focussing on the unique characteristics of multicomponent nanohybrids and their potential use in various applications. The synergistic properties of graphene oxide-gold nanohybrids (GO-Au) are already being used in applications such as biosensing and cancer detection. However, there is currently no standardised protocol for the synthesis of such nanohybrids. Also, an understanding of the fate and toxicity potential of a GO-Au nanohybrid has become pertinent due to their rapid use and resulting inevitable exposure of organisms and the environment. In addition, the possibility of using a metal-doped nanohybrid as chemical tracer for graphene oxide (GO) in environmental and biological systems is interesting for ecotoxicological studies. In this research, GO and GO-Au nanohybrid were synthesised and characterised using several techniques including UV-Vis, TGA, TEM, FTIR, AFM, XPS and Raman. The production of the nanohybrid was repeated a number of times to verify reproducibility of the synthesis protocol. Dispersion stability of the nanohybrid in different environmental media as well as the influence of ageing on its quality were also investigated. A series of assays were performed to assess the toxicity of the nanohybrid on water flea (Daphnia magna). The study successfully generated batches of GOAu nanohybrid that exhibited reproducible characteristics. The nanohybrid also showed good stability in different environmental media and its physicochemical characteristics did not deteriorate over a period of months. The amount of Au in each of the GO-Au nanohybrid samples was highly comparable, suggesting a potential for use as chemical label. Although the nanohybrid did not induce significant acute immobilization or mortality to neonates of daphnia, signs of stress and bioaccumulation were evident from the morphological images of the exposed organisms. The outcome of this research represents a crucial step forward in the development of a standard protocol for the synthesis of GO-Au nanohybrids. It also paves the way towards a better understanding of the nanotoxicity of GO-Au nanohybrid in biological and environmental systems.

Keywords: Ecotoxicity; Nanoparticles; Nanotechnology; Nanosafety

Acknowledgement: This research was funded by the Nigerian government through the Petroleum Technology Development Fund (PTDF) scholarship to T.H.A. and B.I. A.M.Z.d.M and D.S.T.M. thank CAPES and FAPESP foundations for scholarships, respectively, for visiting research at GEES/UoB. The authors are grateful to NANOTOX open-facility at LNNano/CNPEM

V_2O_5-Modified Nb_2O_5: A Versatile Catalyst for Enhanced Photocatalytic Processes

Thaís A. Rodrigues[1], Douglas M. S. Del Duque[2] and Vagner R. Mendonça[1, 2]
[1] Federal University of São Carlos, Science and Technology Center for Sustability, 18052-780, Sorocaba, Brazil; [2] Federal Institute of São Paulo, 18202-000, Itapetininga, Brazil.
thais.rodrigues@estudante.ufscar.br

Population growth has led to various environmental issues, including the contamination of aquatic ecosystems by organic compounds [1] and the release of CO_2 into the atmosphere [2]. One alternative to mitigate these impacts is Heterogeneous Photocatalysis, which utilizes irradiated semiconductors to oxidize organic compounds by generating highly oxidizing radicals like •OH and O_2•- [3] or to reduce CO_2 by converting them into higher value-added products [4]. Since Brazil is the largest Niobium exporter in the world, becomes a political and economic issue for the country to add scientific value to this metal. A way to do that is by applying Nb_2O_5 semiconductor as a photocatalyst. This study aimed to synthesize Nb2O5/V2O5 to promote selectivity in the material. The precursor ammonium niobium oxalate ($NH_4[NbO(C_2O_4)_2(H_2O)_2]\cdot nH_2O$ – CBMM, Brazil) was dissolved in distilled water under vigorous stirring. To this solution, hydrogen peroxide was added at a 10:1 H_2O_2:Nb molar ratio, then 160 mg of V_2O_5 (Synth, 98%) was added and the solution was made up to 130 mL with distilled water and treated in the steel reactor at 150 °C for 24 h. Nb_2O_5 nanoparticles were obtained under the same conditions, reported initially by Leite et al. [5]. The samples were characterized by X-ray diffractometry (DRX), Raman spectroscopy, Fourier-transform infrared spectroscopy (FTIR), and scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDS), and also they were applied in the degradation of rhodamine B dye, in addition, they were applied in the photoreduction of CO_2 in other products with added scientific value, such as CO and H_2, the heterojunction was more selective to the formation of CO than H_2. The results presented that the modification of Nb_2O_5 with V_2O_5 provided enhanced photocatalytic performance in terms of RhB dye degradation and CO_2 photoreduction when compared to the isolated Nb_2O_5, possibly due to the formation of a heterojunction.

[1] T. D. Munusamy, et al., C. S. Yee, M. R. Khan, Adv. Powder Technol. 393, 302 (2014).
[2] L. Collado, et al., Appl. Catal. B 324, 122206 (2023).
[3] S. Gisbertz and B. Pieber, Chem. Photo. Chem. 4, 456 (2020).
[4] J. A. Torres et al., J. CO2 Util. 35, 106 (2020).
[5] E. Leite et al., J. Phys. Chem. B 110, 18088 (2006).

Acknowledgments: This work was supported by CAPES, code finance 001. The authors would like to thank CBMM and Embrapa Instrumentation.

Keywords: niobium; CO2 photoreduction; water treatment.

Ecotoxicological evaluation of Benzotriazole compound in both free and nanoengineered forms

Ralha, T.R.[1]; Abessa, D. M. S.[1]; Perina, F.C.[2]; Martins, R.[2]
[1] UNESP, Campus Litoral Paulista, Departamento de Ciências Biológicas e Ambientais, Instituto de Biociências, Núcleo de Estudos sobre Poluição e Ecotoxicologia Aquática (NEPEA), São Vicente-SP, Brazil; [2] University of Aveiro, Centre of Environmental and Marine Studies (CESAM) & Department of Biology, Aveiro, Portugal.
thaisa.ralha@unesp.br

Introduction: Corrosion represents a concerning problem for metal surfaces exposed to the environment, causing an average loss of 2.5 trillion dollars per year. To mitigate the corrosion damages, several technologies have been employed, such as the use of inorganic salts, cathodic/anionic protection, and chemical inhibitors. Corrosion inhibitors (CI) have been widely used on materials immersed in the sea, but they can be released into the environment and cause toxic effects on biota[1,2] Benzotriazole (BTA) is an important CI; however, it is a persistent compound, resistant to traditional water treatment, and capable of causing hormonal disruption in several organisms[3]. Thus, a new nanoengineered CI is being proposed, consisting of layered double hydroxides (LDH) loaded with BTA, which may be an alternative to efficiently deal with corrosion but causing less environmental impacts. **Objectives:** This project aims to evaluate the toxicity of BTA, in its free and nanostructured forms, to neotropical marine invertebrates. The initial hypothesis of this investigation considers that free BTA is more toxic than its nanostructured form. **Materials and Methods:** Three neotropical marine species are being used: embryos of the sea urchin *Echinometra lucunter*, the sand dollar *Mellita quinquiesperforata*, and the brown mussel *Perna perna*. The toxicity tests assessing the embryolarval development of the aforementioned organisms are performed using internationally standardized protocols[4,5,6] with the objective of establishing the toxic levels of the tested substances (free BTA; BTA-LDH-MgAl, and LDH-MgAl). The results are being analyzed by analysis of variance (ANOVA), followed by Dunnetts' test, in order to determine the Lowest Observed Effect Concentration (LOEC) and No Observed Effect Concentration (NOEC). The results are also analyzed by the Probits method to estimate the effective concentration to 50% organisms (EC50). Further, the data will be used in a larger international project to generate specific distribution curves of sensitivity and determine the environmental hazards of the tested compounds. **Preliminary Results:** The partial results show inconclusive results: for LOEC values, free BTA tends to be less toxic than BTA-LDH-MgAl (100 mg L^{-1} and 33.3 mg L^{-1} respectively). But when the EC50 is analyzed free BTA shows similar or even higher toxicity than the nanostructured form (45.1 (33.5-60.6) mg L^{-1} and 59.9 (21.3 – 168.9) mg L^{-1}, respectively). Because EC50s had very large confidence intervals, more tests are needed to confirm our initial hypothesis.

[1] P. Jain, B. Patidar and J. Bhawsar, J. of B. and Tribo-Corr. 6(2), 1-12 (2020)
[2] J. Tedim et al., ACS Applied Mater. and Interf. 2(5), 1528–35 (2010).
[3] I. Briguglio, S. Piras, P. Corona, E. Gavini, M. Nieddu, G. Boatto and A. Carta, Eur. jour. of med. chem., 97, 612-648 (2015).
[4] ABNT – Associação Brasileira De Normas Técnicas. Ecotoxicologia Aquática. NBR 15350 (2012).
[5] L.C. Mello, T.G. Fonseca, D.M.S. Abessa, Mar. Poll. Bulle., 159 (2020).
[6] ABNT - Associação Brasileira De Normas Técnica. NBR 16456 (2016).

Acknowledgements: This work was supported by Fundação de Amparo à Pesquisa do estado de São Paulo (FAPESP) Proc. Nº 2022/09010-8 and Fundação para a Ciência e a Tecnologia (FCT).

Keywords: benzotriazole, anticorrosives, nanostructured, toxicity.

Development of nanoparticles to vehicle the BotrAMP14 peptide as an alternative for the treatment of bovine mastitis

Thuanny Borba Rios[1,2], Mariana Rocha Maximiano[1,2] and Octávio Luiz Franco[1,2]
[1] S -Inova Biotech, Universidade Católica Dom Bosco, 79117-900, Campo Grande, Brazil; [2] Centro de Análises Proteômicas e Bioquímicas (CAPB)), Universidade Católica de Brasília, 71966-700, Brasília, Brazil.
ocfranco@gmail.com

Bovine mastitis can have a serious impact on milk production chain. Moreover, bovine mastitis may pose risks to public health since the main treatment is the use of antibiotics. Misuse of these antibiotics, in addition to being found as residues in milk, can lead to the emergence of resistance. In this context, the BotrAMP14 peptide was developed from batroxicidin by rational design throughout sequence modifications aimed at improving biological activities and stability. This peptide associated with polymeric nanoparticles is an interesting alternative to circumvent conventional mastitis treatments limitations. Thus, this work aims to obtain and characterize chitosan/sodium alginate nanoparticles for controlled release of the BotrAMP14 peptide, through the ionotropic gelation methodology. The developed nanoparticles were characterized by particle size distribution and zeta potential, in addition to a morphological characterization (SEM). Zetasizer analyzes showed an average nanoparticle size between 300 and 400 nm, which was confirmed by SEM analyses. Zeta potential studies showed that the particles have positive surface charges, with values close to + 30 mV. Furthermore, the peptide encapsulation efficiency was evaluated, which was high, with values exceeding 90%, as well as the *in vitro* release, which presented a profile divided into two phases. The first release phase showed a constant release rate up to 18h. Alter this period, the second phase showed a faster release, reaching 70 % of peptide released at the end of 24h. Finally, the *in vitro* antimicrobial assay to determine the minimum inhibitory concentration (MIC) indicated growth inhibition of *Staphylococcus aureus* growth, one of the main etiological agents of bovine mastitis. Finally, the results obtained so far demonstrate that the nanoparticulate system containing the BotrAMP14 peptide has the potential to be used as an alternative to antibiotics in the treatment of mastitis.

Keywords: antimicrobial peptide; nanobiotechnology; polymeric nanoparticles; bovine mastitis

Monitoring the effects of solar radiation in a 3D in vitro model of skin by Raman spectroscopy

Lopez-Gonzalez. Ulises[1], Casey. Alan[2] and Byrne. Hugh, J.[2]
1 Universidad de Monterrey, Physics and Mathematics deparment, 66238, Monterrey, Mexico; 2 FOCAS Research Institute, Technological University Dublin (TUD) , Nanolab, D8, Dublin, Ireland.
Ulises.lopezg@udem.edu

Understanding the interaction between solar radiation and skin barrier is critical in preventing the ocurrance of skin cancer. [1] Multiple studies have been performed in 2D cell culture models under simplified and unrealistic conditions. 3D culture models better mimics the complexity and morphology of in vivo conditions, although the effects of the 3D extracellular matrix have not been well studied. [2] Monitoring the instantaneous biochemical and celular response to exposure, and the influence of the 3D environment, could provide an enhanced understanding of the fundamental processes of photocarcinogenesis. This work presents an analysis of the biochemical impacts of simulated solar radiation (SSR) occurring in immortalised human epithelial keratinocytes (HaCaT), in a 3D skin model, compared to 2D culture. Cell viability was monitored using the Alamar Blue colorimetric assay (AB), and the impact of the radiation exposure, at the level of the biomolecular constituents (nucleic acids and proteins), were evaluated through the combination of Raman microspectroscopy and multivariate statistical analysis. The results suggest that SSR exposure induces alterations of the conformational structure of DNA as an immediate impact, whereas changes in the protein signature are primarily seen as a subsequent response.

[1] Gargotti, M., Lopez-Gonzalez, U., Byrne, H.J. et al. Cytotechnology (2018) 70: 261. https://doi.org/10.1007/s10616-017-0139-7).
[2] A. Tfayli, O. Piot, F. Draux, F. Pitre, M. Manfait, Biopolymers 2007, 87(4), 261.

Acknowledgements: This work was funded by Consejo Nacional de Ciencias y Tecnologia (CONACYT), Mexico. Open access funding provided by IreL. The authors would like to thank the University of Monterrey (UDEM) and the SPSAS NanoAgri& Enviro school of sciences.

Keywords: Raman Spectroscopy, 3D skin model, Simulated solar radiation

Nanoformulation of metribuzin herbicide to environmental risk reduction and improvement of weed control

Vanessa Takeshita[1], L.B. Carvalho[2], J.A. Galhardi[2], G.V. Munhoz-Garcia[1], B.C. Cardoso[1], C.W. Pinácio[1], R.F. Pimpinato[1], H.C. Oliveira[3], V.L. Tornisielo[1] and L.F. Fraceto[2]

1 Center of Nuclear Energy in Agriculture, University of São Paulo, 13.416-000, Piracicaba, Brazil; 2 Institute of Science and Technology, São Paulo State University, 18.087-180, Sorocaba, Brazil; 3 State University of Londrina, 86.057-970, Londrina, Brazil.

vanessatakeshita@usp.br

Nanoencapsulation of herbicides could be an excellent alternative as a carrier to reduce losses in the environment and improve weed control efficacy. Metribuzin is a pre-emergent herbicide, presents highly mobile in the soil, and is non-persistent. A nanoformulation is to metribuzin herbicide can reduce leaching, and increase availability for weed control, with low environmental risk. In this study, the aim was to understand the behavior of metribuzin nanoformulation (*nano*MTZ), based on a biodegradable polymeric nanoparticle, in the soil and plant system. The stability of nanoparticles was monitored per 120 d. We investigated the physiological parameters and weed control efficacy of *Ipomoea grandifolia* plants. In the soil, we analyze the fate and mobility of nanoformulation in different soils, followed by the effects on soil enzymatic activity. Weed control was effective even at the lowest dose of *nano*MTZ (48 g a.i. ha^{-1}), compared to the conventional herbicide in inhibiting PSII activity and decreasing pigment levels. No differences were verified in the half-life of *nano*MTZ when compared to a commercial formulation of the herbicide, and suppressive effects on soil enzymatic activities were not observed. The retention of *nano*MTZ in the soil was lower than in commercial formulation. However, the mobility of *nano*MTZ was not significantly increased, reflecting a low risk of groundwater contamination. Overall, we verified the great stability of the metribuzin nanoformulation over time, improvement in efficacy, and low environmental risk for the metribuzin nanoformulation. As complementary gains, we showed the radiometric technique, to track metribuzin in the soil, as an important method for environmental behavior tests.

Acknowledgements: This work was supported by São Paulo Reasearch Foundation (Process #2019/04758-1; Process #2022/00509-0; #2018/23608-8; #2022/00718-8; #2017/21004-5; #2017/15220-7), Conselho Nacional de desenvolvimento Científico e Tecnológico (CNPq), Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Capes (PrInt/Capes #88887.468162/2019-00), Associação dos Produtores de Soja e Milho do Estado de Mato Grosso (APROSOJA - Projeto Agrocientista), and Instituto Mato-Grossense do Agronegócio (IAGRO - MT).

Keywords: nanoherbicide, weed control, environmental risk, environmental fate

Uptake and translocation of ZnO@MSN in tomato plant following foliar application

Xiaoyu Gao, Anirban Kundu, Vinicius Bueno, Arshath Abdul Rahim, Subhasis Ghoshal
Department of Civil Engineering, McGill University, H3A 0C3, Montreal, Canada
Email_corresponding_author@subhasis.ghoshal@mcgill.ca

Mesoporous silica-based nanocarriers (MSN) can provide controlled and sustained micronutrient delivery to food crops, as well as being highly biocompatible. Through a more targeted foliar application approach, it can potentially reduce energy consumption and eliminate soil and water pollution. However, the uptake and translocation of nanocarriers encapsulated micronutrients have not been demonstrated. The objectives of this study were to compare the efficiency of Zn uptake using core-shell ZnO nanoparticles encapsulated in a nano-sized mesoporous SiO_2 nanoshell (ZnO@MSN) to bare ZnO nanoparticles (ZnO NPs), and Zn salt ($ZnCl_2$) to tomato plant, *Solanum lycopersicum*, and to assess the particulate translocation of ZnO@MSN to different plant parts. In this study, ~70 nm ZnO@MSN with ~30 nm ZnO NP core were synthesized for delivery of Zn to plants by foliar uptake. In a model plant media (pH = 5), compared to the rapid dissolution of bare ZnO NPs (90% Zn dissolution after 4 h), ZnO@MSN released Zn at a slower rate (40% Zn dissolution after 3 weeks). The slow and controlled release of ZnO@MSN enabled a sustained Zn delivery over a longer period. 40 μg of Zn micronutrient of either ZnO@MSN suspension, ZnO NPs suspension, or $ZnCl_2$ solution was deposited on a single leaf after 2 weeks of a growth period for different Zn treatments. For ZnO NPs treatment, no Zn uptake was observed after 2 days of dosing. For $ZnCl_2$ treatment and ZnO@MSN treatment, similar amounts of Zn uptake and translocation to upper leaves, and shoots were observed 2 days after dosing (15.5 ± 2.4 μg Zn and 11.4 ± 2.2 μg Zn for $ZnCl_2$ treatment and ZnO@MSN treatment, respectively). Most ZnO@MSN were translocated in plants in their particulate form as evident from single particle inductively coupled plasma mass spectrometry measurement on different plant parts and transmission electron microscopy analysis on the cross-section of the dosed leaf. These results suggest that the MSN enhanced the uptake of ZnO NPs in tomato plants. ZnO@MSN had a better delivery efficiency compared to bare ZnO NPs and is likely to be able to provide Zn over a significant period of the plant growth period, reducing the need for multiple applications.

Acknowledgments: This work was supported by funding support from the Natural Sciences and Engineering Research Council of Canada (grant nos. RGPIN-2016-05022 and STPGP 506450-17), the Fonds de Recherche du Québec–Nature et Technologies (grant no. 286120) and the Canadian Foundation for Innovation. V.B. and A.K. were supported in part by McGill Engineering Doctoral Awards. The authors thank Dr. Hojatollah Vali, Dr. S Kelly Sears, Jeannie Mui, and David Liu, Facility for Electron Microscope Research (FEMR), McGill University for their assistance with TEM analyses.

Keywords: ZnO nanoparticles, mesoporous SiO2 nanoparticles, foliar application, micronutrient delivery

Singlet Molecular Oxygen Generation *via* Unexpected Emission Color-Tunable CdSe/ZnS Nanocrystals for Applications in Photodynamic Therapy

Zahid U. Khan[1,2], Latif U. Khan[2,3], Hermi F. Brito[3], Magnus Gidlund[4] and Paolo Di Mascio[1]
1Department of Biochemistry, Institute of Chemistry, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil.
2Department of Fundamental Chemistry, Institute of Chemistry, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil.
3Synchrotron-light for Experimental Science and Applications in the Middle East (SESAME) P.O. Box 7, Allan 19252, Jordan.
4Department of Immunology, Institute of Biomedical Sciences-IV, University of São Paulo (USP), 05508-000, São Paulo-SP, Brazil.
Corresponding Emails: pdmascio@iq.usp.br, zahid@iq.usp.br

It is highly desirable in biomedical sciences to utilize the multifunctional nanoparticles of similar size with tunable emission. Since the optoelectronic properties of quantum dots (QDs) originate from size-dependent quantum confinement effects; therefore, we developed an alternate approach to synthesize color-tunable CdSe/ZnS QDs based on interfacial ion exchange (predominantly exchange of Se2- by S2- anion), using 1-dodecanthaiol (DDT) and oleylamine (OLA) solvents system as a sensitive parameter. The wide-range color-tunability (490-570 nm) was achieved unexpectedly as result of interfacial alloying without a significant change in the size (from 4.45 to 4.81 nm) of QDs, as confirmed by XAFS data analysis. Owing to the molecular-like sensitization behavior, the QDs were evaluated for singlet molecular oxygen (1O2) efficiency. They were further studied in RAW macrophages for biocompatibility, bioimaging and delivering pathways to use for future photodynamic therapy (PDT). The QDs demonstrated efficient singlet molecular oxygen (1O2) quantum yields (ΦQDs) of 14, 12, and 18% for yellow-emitting CdSe/ZnS QDs **(I)**, green-emitting CdSe/ZnS QDs **(II)**, and blue-emitting CdSe/ZnS QDs **(III)**, respectively. The QDs treated cells presented high cell viability above 85% and induced no cell activation. Fluorescence and TEM images of cells manifested considerable amount of QDs in the intracellular regions. The pathway-specific inhibition measurements revealed that the QDs were internalized by cells *via* energy-dependent endocytosis predominantly macropinocytosis and other lipid raft-mediated endocytic pathways and accumulated presumably in endosome/lysosomes. This study will open new possibilities of band edge engineering and pathway-specific delivery of QDs-based theranostic into a site of interest for simultaneous bioimaging and photodynamic therapy.

Keywords: Quantum dots, Ion exchange, Color-tuning, Singlet molecular oxygen generation, Cellular labeling, Cellular uptake mechanism.

Nanoparticles fate on plant leaves: Understanding entry mechanisms

M. Wagner[1], A. Avellan[1] and C. Larue[2]
1 Géosciences Environnement Toulouse (GET), CNRS, Toulouse, France; 2 Laboratoire Ecologie Fonctionnelle et Environnement, CNRS, Toulouse, France
mickael.wagner@get.omp.eu

Nanotechnologies could help to meet the critical needs for a more responsible and sustainable agriculture. Yet, knowledge about the complex interactions between plants and nanoparticles (NPs) are style scarce, especially at the foliar interface, although it is a major surface used for plant protection. Especially, the possible entry and internalization mechanisms of NPs in leaves remain unclear. Hypothesized entry are stomata, trichomes, cuticle and hydathodes pores. This poster presents the fate of bioavailable NPs at the leaf interface depends on known and hypothetical drivers. Firstly, physical-chemical properties of NPs drive their behavior. Hydrophobicity should favor cuticle crossing. Secondly, various plant leaf structures offer different entry routes that should contribute differently to NPs uptake. In my Ph.D., I plan to use Arabidopsis thaliana loss/gain of function mutant to test if the over or under expression of a structure leads to variations in NP absorption. However, before proceeding it is crucial to establish a reliable method for distinguishing between leaf ab- and ad-sorption. To date, only one study has tested the effectiveness of the conventional ethanol/HNO3 sequential rinsing removing adsorbed NPs without damaging the leaves. These experiments will advance our knowledge of NP entry pathways into leaves and suitable study methods. They will also enable to test the downward transfer of NPs after foliar exposure. This will constitute an additional step to study the mechanisms of translocation of NPs among plant compartments as well as the possible associated transformations. Overcoming this gap in knowledge will allow to think more precisely about the delivery mechanism of micronutrients by NPs needed to design a sharp and responsible agriculture.

Keywords: Nanoparticle, leaf, adhesion, uptake

Developing a predictive model for nanomaterial toxicity in *Daphnia magna* under different environmental conditions

Katie Reilly[1], Marta Swirog[2], Ewelina Wyrzykowska[3], Thomasz Puzyn[2], Thomas Exner[4] and Iseult Lynch[1]

[1]University of Birmingham, United Kingdom, [2]QSAR Lab Ldt., Poland, [3]University of Gdansk, Poland, [4]Seven Past Nine

k.reilly.1@bham.ac.uk

Environmental conditions are being recognized as important parameters to consider during nanomaterial (NM) toxicity testing due to NMs responsiveness to their specific local environments. NM transformations in the environment based on biotic and abiotic factors make them an interesting and challenging material to assess. However, currently Test Guidelines (TGs) are designed to priorities the ability to compare the end points and reproduce the test conditions to enable ranking of toxicants of concern. Due to the variable nature of environmental conditions such as natural organic matter content, these factors are often explicitly removed from the test design. For example, the OECD 202 (Daphnia acute toxicity test) stipulates that natural organic matter (NOM) should be excluded from the test medium due to the heterogeneous nature of NOM. However, NOM has been previously shown to have a potential stabilizing effect on NM, and can be used as a more natural method of ensuring particles remain dispersed (minimizing the agglomeration) and therefore has the potential to significantly impact the NM stability during the test period making this an important parameter to consider for environmental assessments. Daphnia magna are a fantastic model organism to explore these potential impacts, as they have historically been used for a range of chemical, and more recently nanomaterial and microplastic effects [1]. Daphnia have transparent body which makes then an ideal model for particulate based work, and they also have rapid clonal reproduction and filter feed which enables a range of toxicants and responses to be explored. In this study, the media used for toxicity testing varied in pH, NOM content and ionic strength (such as changes in the salt content such as sulphides) which enabled a range of potential environmental drivers to be assessed. The nanomaterial toxicity was explored in the different media to enable the variation in response to be determined, and links between the NM and the medium to be determined to enable predictions for toxicity going forwards based on the physico-chemical parameters [2]. Additionally, this work was used as a case study for the development of an instance map to visualise the experimental workflow, the points (or instances) at which the NMs are likely to transform such as dispersion in the test medium and ingestion by the Daphnids. The instance map linked to data capture templates to ensure that all of the relevant metadata was also captured to facilitate model development and data reuse going forwards in line with FAIR data principles.

[1] Karatzas et al. Small. 16,36. (2020). doi.org/10.1002/smll.202001080
[2] Swirog et al. Sci. Total Environ. 840. (2022) doi.org/10.1016/j.scitotenv.2022.156572

Acknowledgements: This work was funded through a collaboration of several projects: RiskGONE (Grant Agreement nº 814425), NanoSolveIT (Grant Agreement nº 814572) and CompSafeNano (Grant Agreement nº 101008099)

Keywords: Daphnia magna, natural organic matter, nanotoxicity.

pages.cnpem.br/spsasnano