



PRESSYNC
*Synchrotron Techniques
Under High Pressure*

July 31st to August 2nd
2019

ABSTRACT BOOK



MINISTRY OF
SCIENCE, TECHNOLOGY,
INNOVATION AND COMMUNICATION





Organization



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Foreword

Between July 31st and August 2nd, 2019, the Brazilian Synchrotron Light Laboratory (LNLS), part of the Brazilian Center for Research in Energy and Materials (CNPEM) located at Campinas (SP), is hosting the event Synchrotron Techniques Under High Pressure (PRESSYNC).

PRESSYNC is a satellite workshop to the 27th International Conference on High Pressure Science and Technology (AIRAPT27).

The AIRAPT27 conference, sponsored by AIRAPT (International Association for the Advancement of High-Pressure Science and Technology), is the largest and most important international scientific event in the field of high-pressure science and technology.

The 27th conference in Rio de Janeiro will be the first one to be held in the southern hemisphere. The conference gathers a multidisciplinary international community whose focus is on fundamental and applied research at extreme pressure conditions, as well as on the associated technology and instrumentation.

Taking advantage of this opportunity, the PRESSYNC Satellite Workshop will bring together world leaders in high-pressure science to discuss the potential of synchrotron-based techniques under high pressure on the new fourth-generation synchrotron light sources, such as Sirius.

Sirius, the new Brazilian synchrotron light source, is planned to be one of the most advanced facilities of its kind in the world, opening new perspectives for research in a wide range of fields. Hence, PRESSYNC aims specially to motivate the community around the several possibilities that will be available at Sirius' extreme conditions beamline, EMA.





Program at a glance

	July 31 st	August 1 st	August 2 nd
8:30 - 9:00	<i>Registration</i>	--	--
9:00 - 10:20	<i>Chair: Y. Petroff</i> H. Westfahl N. Souza-Neto	<i>Chair: D. Haskel</i> A. Grockowiak A. Ayala	<i>Chair: J.-P. Itie</i> K. Dziubek F. Gervasoni
10:20 - 11:00	<i>Coffee Break</i> Discussions	<i>Coffee Break</i> Discussions	<i>Coffee Break</i> Discussions
11:00 - 13:00	<i>Chair: H. Tolentino</i> J.-P. Itie E. Granado A. Gomes	<i>Chair: N. Souza-Neto</i> G. Hearne P. Tarso H. Liu	<i>Chair: E. Granado</i> N. Balzaretti G. Fabbris C. Adriano
13:00 - 14:40	<i>Lunch</i> Thematic Discussions	<i>Lunch</i> Thematic Discussions	<i>Lunch</i> Thematic Discussions
14:40 - 16:00	<i>Chair: P. Pagliuso</i> D. Haskel P. Rosa	<i>Chair: C. Adriano</i> E. Bittar S. Tozer	<i>Chair: H. Westfahl</i> K. Shimizu S. Deemyad
16:00 - 16:40	<i>Coffee Break</i> Poster Session Discussions	<i>Coffee Break</i> Poster Session Discussions	General discussions
16:40 - 18:00	<i>Chair: G. Fabbris</i> F. Alabarse V. Prakapenka	<i>Chair: R. Reis</i> M. Einaga M. Nicklas	
		Workshop dinner	Workshop Ends and departures



Detailed Program - Wednesday, July 31st, 2019

08:30 - 9:00 **Opening/Registration**

Chair: Yves Petroff

09:00 - 09:40 **Harry Westfahl** – *Brazilian Synchrotron Light Laboratory – Brazil*
“Sirius: The new Brazilian Synchrotron Light Source”

09:40 - 10:20 **Narcizo M. Souza-Neto** – *Brazilian Synchrotron Light Laboratory – Brazil*
“EMA: Extreme conditions beamline @ Sirius”

10:20 - 11:00 **Coffee Break**

Chair: Helio Tolentino

11:00 - 11:40 **Jean-Paul Itie** – *Synchrotron Soleil – France*
“The use of wiggler white beam: new opportunities for high pressure science”

11:40 - 12:20 **Eduardo Granado** – *University of Campinas – Brazil*
“First-order structural transition and pressure-induced lattice/phonon anomalies in Sr₂IrO₄”

12:20 - 13:00 **Antonio Gomes** – *Federal University of Ceara – Brazil*
Resonance Raman spectroscopy in strained nanosystems

13:00 - 14:40 **Lunch time**

Chair: Pascoal Pagliuso

14:40 - 15:20 **Daniel Haskel** – *Argonne National Laboratory – USA*
“Magnetic scattering and spectroscopy at high pressures at APS and APS-U”

15:20 - 16:00 **Priscila Ferrari Rosa** – *Los Alamos National Laboratory – USA*
“The dawn of topology in condensed-matter physics”

16:00 - 16:40 **Coffee Break and Poster Sessions**

Chair: Gilberto Fabbris

16:40 - 17:20 **Frederico Alabarse** – *Elettra Sincrotrone Trieste – Italy*
“High pressure activity at Elettra Sincrotrone Trieste and its new dedicated high-pressure diffraction beamline – Xpress”

17:20 - 18:00 **Vitali Prakapenka** – *University of Chicago – USA*
“Advanced synchrotron and optical techniques for mineral characterization and synthesis”



Detailed Program - Thursday, August 1st, 2019

Chair: **Daniel Haskel**

09:00 - 09:40 **Audrey Grockowiak** – *National High Magnetic Field Laboratory – USA*
“Extreme conditions measurements in high magnetic fields”

09:40 - 10:20 **Alejandro Ayala** – *Federal University of Ceara – Brazil*
“Low dimensional halide perovskites under extreme conditions”

10:20 - 11:00 **Coffee Break**

Chair: **Narcizo Souza Neto**

11:00 - 11:40 **Giovanni Hearne** – *University of Johannesburg – South Africa*
“Magnetic-electronic studies at a megabar: the new frontier”

11:40 - 12:20 **Paulo de Tarso C. Freire** – *Federal University of Ceara – Brazil*
“High-pressure study of L-leucyl-L-leucine hydrate”

12:20 - 13:00 **Haozhe Liu** – *Center for High Pressure Science & Technology Advanced Research – China*
“High pressure researches using multiple synchrotron X-ray techniques”

13:00 - 14:40 **Lunch time**

Chair: **Cris Adriano**

14:40 - 15:20 **Eduardo Bittar** – *Brazilian Center for Research in Physics – Brazil*
“Charge density wave quantum phase transitions studied by x-ray diffraction”

15:20 - 16:00 **Stan Tozer** – *National High Magnetic Field Laboratory – USA*
“Unraveling structural and electronic properties to elucidate function—on the feasibility of simultaneous high pressure, high magnetic field X-ray scattering and fermiology studies”

16:00 - 16:40 **Coffee Break and Poster Sessions**

Chair: **Ricardo Reis**

16:40 - 17:20 **Mari Einaga** – *Osaka University – Japan*
“Synthesis and Multiple-Physical Property Measurements under Extreme Conductions in Synchrotron Facility SPring-8”

17:20 - 18:00 **Michael Nicklas** – *Max Planck for Chemical Physics of Solids – Germany*
“Tuning competing ground states in geometrically frustrated low-dimensional systems”



Detailed Program - Friday, August 2nd, 2019

Chair: **Jean-Paul Itie**

09:00 - 10:20 **Kamil F. Dziubek** – *Institute of Chemistry of OrganoMetallic Compounds – Italy*
“High pressure syntheses of selected binary inorganic compounds from elements”

10:20 - 11:00 **Fernanda Gervasoni** – *Federal University of Goiás – Brazil*
“From Earth’s crust to mantle: high pressure techniques to solve geoscience questions”

10:20 - 11:00 **Coffee Break**

Chair: **Eduardo Granado**

11:00 - 11:40 **Naira Balzaretti** – *Federal University of Rio Grande do Sul – Brazil*
“Ex-situ analyses of large volume high-pressure experiments using LNLS facilities: some examples”

11:40 - 12:20 **Gilberto F. L. Fabbri** – *Argonne National Laboratory – USA*
“Resonant Inelastic X-ray Scattering at High Pressure: Challenges and Opportunities”

12:20 - 13:00 **Cris Adriano** – *University of Campinas – Brazil*
“Spin rotation induced by applied pressure in Cd-doped Ce₂RhIn₈ heavy fermion compound”

13:00 - 14:40 **Lunch time**

Chair: **Harry Westfahl**

14:40 - 15:20 **Katsuya Shimizu** – *Osaka University – Japan*
“Investigation of electrical conductivity of hot dense hydrogen: experimental background enabling this”

15:20 - 16:00 **Shanti Deemyad** – *University of Utah – USA*
“Metastable and ground state structures of lithium under pressure”

16:00 - 18:00 **General Discussion/Workshop Ends**



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ABSTRACTS



CNPq

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Poster Presentation

All-electron and pseudopotential DFT calculations of rhenium equation of state in the terapascal regime

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Rhenium is often used as a metal gasket in high-pressure experiments with the diamond-anvil cell, in which the gasket itself can be used to estimate P by x-ray diffraction at the point of contact with the sample. The pressure is then obtained from the equation of state (EOS) of the gasket's material [1]. The EOS of hcp rhenium has been previously determined up to 1.5 TPa ($V/V_0 \sim 0.46$) using all-electron (AE) density functional theory (DFT) including core relativistic effects [2]. This work focuses on exploring the influence of core electrons on the EOS of Re above 1 terapascal (TPa) by comparing results obtained using pseudopotentials (PPs) with previous AE calculations. DFT calculations were performed using fully relativistic PPs with Quantum Espresso [3]. We tested two norm-conserving PPs generated with the optimized Vanderbilt approach, one using the PBE exchange-correlation functional [4] and the other, more recently developed, using PBEsol [5]. The calculations were performed using the PBEsol exchange-correlation functional and the same conditions of the previous AE study, where applicable. Both PPs yielded results in good agreement with AE calculations. In particular, we observe a nonmonotonic variation of the c/a ratio with the pressure that agrees very well with the AE results. The fitted parameters of the Vinet EOS, the bulk modulus B_0 (380(2) GPa and 379(2) GPa for the PBE and PBEsol PPs, versus 377(5) GPa for AE), and its pressure derivative B_0' (4.58(1) and 4.59(1) for the PBE and PBEsol PPs, vs. 4.62(3) for AE), are identical (considering the uncertainties). The results differ mostly for the equilibrium volume at zero pressure, V_0 (196.7(3) \AA^3 and 199.2(1) \AA^3 for PBE and PBEsol PPs, vs. 195.2(3) \AA^3 for AE). For a given V/V_0 ratio, the pressures estimated using the EOSs derived from the PPs and AE calculations are in very good agreement, thus suggesting that the PPs used in this study are well suited even at such high compression regime.

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Acknowledgement

The support from the Brazilian agencies Coordenação de Aperfeiçoamento de Pessoal de Nível Superior - Brasil (CAPES), grant 88887.311575/2018-00, and Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq) - grant 304831/2014-0 (CAP).



Poster Presentation

Effect of pressure on nanostructured a Bi_3Ni produced by mechanical alloying

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Studies of binary compounds incorporating Bismuth have attracted the attention of several researchers because it presents unusual properties in the creation of exotic materials. Binary Ni (Ni) and bismuth (Bi) alloys are materials with various applications such as intermetallic layers, galvanization of steels against atmospheric corrosion, lead-free solder, superconductivity, etc. Bi_3Ni is an intermetallic compound with properties which promote the material to an excellent thermoelectric [1], superconducting with $T_c = 4.06$ K and presents the coexistence of superconductivity and ferromagnetism [2]. In this work, we study the pressure effect of up to 30 GPa in the intermetallic compound Bi_3Ni (Pnma structure) nanostructured by mechanical milling after 19 hours of milling. Through dispersive X-ray diffraction (ADXRD) measurements in situ the ADXRD standards were followed by Rietveld refinement. The volume versus pressure data were fitted to a third order Birch-Murnaghan equation [3] and the value of the module $B_0 = 38$ (2) GPa was obtained.

References

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Acknowledgement

We acknowledge the financial support from the Brazilian funding agency CAPES. We thank the Brazilian Synchrotron Light Laboratory - LNLS.



Poster Presentation

High pressure Raman scattering of DL-isoleucine crystals and DFT calculations

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Pressure-dependent studies of amino acids crystals have been performed for more than two decades. In this work we will show the results obtained on the amino acid DL-isoleucine by means of Raman spectroscopy and DFT calculations. DL-isoleucine single crystals were grown by the slow evaporation method at ambient temperature. Their vibrational properties were studied at ambient temperature as a function of pressure by Raman scattering. At ambient conditions the mode assignment was done in terms of the Potential Energy Distribution (PED) through density functional theory calculations. The pressure-dependent investigation shows modifications in the Raman spectra recorded between 30 and 3200 cm⁻¹ that were interpreted as phase transitions undergone by the crystal between 1.3 and 1.9 GPa and between 3.6 and 5.1 GPa. Finally, stress was simulated on the unit cell of the crystal from ambient up to 5.0 GPa.



Poster Presentation

High pressure researches using multiple synchrotron X-ray techniques

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In this presentation, we would like to show the selected high pressure researches using various synchrotron X-ray techniques, including X-ray diffraction and scattering method, inelastic and spectroscopy techniques, imaging techniques, time resolved techniques. The pressure induced phase transition for crystalline and non-crystalline cases would be introduced. The application of imaging techniques, especially 3D tomography method to determine non-crystalline sample density change, would be highlighted. Charge transfer behavior, phase transition patterns upon strong compression, and phase stability at various compression rate will be mentioned briefly.



Poster Presentation

Hot-pressed Silicon Carbide and Aluminum Nitride for Synchrotron Light Sources

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Synchrotron light sources are large machines, designed to produce the synchrotron light, with the function of unveiling molecular and electronic structures of different materials in order to understand their fundamental properties [1]. These machines operate in ultra-high vacuum atmosphere, requiring specific properties for all the devices used on it, like vacuum tightness, low thermal expansion coefficient, high density and good thermal shock resistance. Silicon carbide (SiC) and aluminum nitride (AlN) are some of the ceramic materials that comply with these properties [2,3]. Both SiC and AlN are materials that require preferably pressure-assisted sintering process and inert atmosphere to produce dense ceramic components with low or none open porosity, a necessary characteristic to reach adequate vacuum tightness. Hot pressing is the most common technique where pressure is applied along with temperature rise during sintering cycle for industrial purposes [4-7]. In this work ceramic pieces of SiC and AlN were produced by hot pressing at 1900 and 1700°C, respectively, using Y₂O₃ as sintering aid. Characterization tests were done in the ceramic parts obtained for identification if the requirements for their application in ultra-high vacuum were achieved.

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Acknowledgement

FAPESP, Finep, Engecer.



Poster Presentation

Influence of hydrostatic pressure on the crystalline structure of Fe₂MnSi Heusler compound

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Heusler system of compounds manifest extremely interesting magnetic and structural properties [1]. Extensive theoretical and experimental works verified that their physical properties are strongly correlated with their crystalline structural properties [2]. Then any control parameters such as pressure and temperature, that influences the latter properties are expected to have an impact on the properties of the former. Here in this work, we are interested in investigating the baric evolution of the structural parameters of the Heusler compound Fe₂MnSi. For this purpose, we performed Synchrotron X-ray diffraction measurements on a polycrystalline sample of Fe₂MnSi which was subjected to various pressures ($0.2 \leq P \leq 40$ GPa) and to the following selected temperatures 30, 120 and 300 K. All studied isothermal and isobaric diffractograms are found to manifest a stable cubic structure. Furthermore, Murnaghan analysis of experimental data yield parameters that are compatible with the values found in the literature [4]. We discuss the possible magneto-structural coupling in this class of materials.

References

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Acknowledgement

This work was supported by the Brazilian agency CNPQ. SXRD were measured at the Brazilian Synchrotron Light Laboratory (LNLS), Campinas, Brazil. We thank Bruno Pimentel (UFF) for the assistance during the performing the SXRD measurements.



Poster Presentation

Nanocrystalline Nickel Sulfide prepared by mechanochemistry and evaluated under high-temperature and high-pressure conditions

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Nanocrystalline Nickel Sulfides have been prepared mechanochemically in our lab using ball milling in an inert atmosphere at room temperature, starting from $\text{Ni}_x\text{S}_{100-x}$ powder mixtures. X-ray powder diffraction (XRPD) was used to investigate the structural and microstructural evolution of the Nickel Sulfides with milling time. The formation of trigonal Ni_3S_2 phase (space group R32H) starting from $\text{Ni}_{60}\text{S}_{40}$ powder mixture occurs with only 1.5 h, remaining stable up to 24 h of milling. The cell volume, lattice parameters, atomic coordinates and isotropic atomic displacement (thermal) parameters of the Ni_3S_2 phase, as well as its average crystallite size and micro-strain, were determined from Rietveld analysis of the XRPD data. The average crystallite size decreases from about 37 nm to 22 nm with milling time increasing. The microstrain also decreases with milling time increasing. The high-temperature experiments showed that the melting point of the nanocrystalline Ni_3S_2 is about 660°C, which is much lower than bulk. Transmission electron microscopy (TEM) images and electron diffraction patterns confirmed the nanometric size of the crystalline domains but revealed that it belongs to larger agglomerated particles (~100 nm). The nanocrystalline samples have their magnetic properties characterized by vibrating sample magnetometer (VSM), showing an evolution from ferromagnetism to a mixed magnetic state as milling time increases. The high-pressure experiments revealed no phase transitions up to 20 GPa and a bulk modulus of about 143 GPa for the Ni_3S_2 nanophase using the least-squares fit of first-order Murnaghan equation of states.

Acknowledgement

We are grateful to the Brazilian agencies CNPq, CAPES and FAPESC for financial support. The XRPD, VSM and TEM/SAED/EDS measurements were performed at Laboratório de Difração de Raios-X (LDRX), Laboratório Multiusuário de Caracterização Magnética de Materiais (LabCAM) and Laboratório Central de Microscopia Eletrônica (LCME) multiuser facilities at UFSC.



Poster Presentation

Pair Distribution Function Analysis applied to nanostructured FeSb₂ under high-pressure

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FeSb₂ is a narrow gap semiconductor that has been drawn considerable attention recently due to the observation of a very high thermoelectric power [1]. Under ambient conditions, this compound crystallizes in an orthorhombic structure. In a previous study [2], we reported the nucleation of a tetragonal FeSb₂ phase for pressures above 14.3 GPa. In this work, the main goal is elucidation of the structural changes promoted by high-pressure on FeSb₂ from an approach that combining the Rietveld method and pairs distribution function analysis. The results obtained can give support to understand the improvement in thermoelectric properties this compound. The application of this approach permitted following the effect of high pressure on the $G_{\text{Fe-Fe}}(R)$, $G_{\text{Fe-Sb}}(R)$ and $G_{\text{Sb-Sb}}(R)$ functions, as well to determine which atomic pairs are most affected. The first coordination shell of $G_{\text{Sb-Sb}}(R)$ correlations is specially affected with increased pressure. From the coordination numbers for the first neighbors, the Cowley-Warren chemical short-range order parameter (α_{CW}) was calculate. A value $\alpha_{\text{CW}}=0.13$ was obtained, indicating that there is preference for forming homopolar pairs or clusters in the first coordination shell.

References

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Acknowledgement

The authors acknowledge the Brazilian funding agency CAPES for the financial support.



Poster Presentation

Phase transformations of the Bm form of octadecanoic acid studied through Raman scattering

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Fatty acids (carboxylic acids) have interesting physical chemical properties and with high melting enthalpy, being good candidate to applications in energy storage and phase change materials technologies. As well as most the majority of organic materials, carboxylic acids in crystalline phase show polymorphism, which is a solid state phenomenon related to the difference in molecular conformation in crystalline structure. The diversity of possible crystalline forms at carboxylic acids depends of the chain length, parity and number of unsaturation in alkyl chain. Specifically to the chain parity, to date, it was observed for even normal fatty acids the forms A1, A2, A3, Asuper, C, Bo/m, Eo/m [1]. It is reported in the literature that the stearic-acid crystal in the C form (monoclinic) has undergone a series of pressure-induced phase transformations at several pressure values [2]. On the other hand, the question arose as to would be the thermodynamic behavior of other stearic-acid polymorphic phases under non-ambient pressure conditions. In this work, the stability of stearic-acid crystal in the Bm form at pressures varying from 0.0 up to 5.9 GPa through Raman scattering is reported. The behavior of the Raman modes indicates that the crystal undergoes two of phase transformations. The first change as observed at around 0.4–0.8 GPa range which was associated with modifications in the lattice (external) vibrations and CH₂ rocking vibrations. The second change was noted between 2.7 and 4.8 GPa due to spectral modifications that occurred at almost all external and internal modes which were associated with a structure modification or rearrange in the configuration of the dimers.

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Acknowledgement

All authors thank the MCT/CNPq and CAPES Public Notices.



Poster Presentation

Phase Transitions of Styrene-Butadiene-Styrene Thin Films Induced by High Pressure Carbon Dioxide

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In this work, we study the influence of supercritical carbon dioxide (Sc-CO₂) on the phase behavior of a cylinder forming polystyrene-block-polybutadiene-b-polystyrene (SBS) triblock copolymer thin film. Solvent annealing with Sc-CO₂ (at 40°C and 90 bar) can produce patterns with long-range order. These patterns become unstable for thin films with a small thickness. These results are in good agreement with self-consistent mean field calculations, which indicates that a dewetting transition occurs for thickness below the radius of gyration of the molecule, due to long-range Van der Waals interactions. After decompression and solvent extraction, the initially swelled polymer nanostructure suffers a strong reduction in the average domain spacing, which has a deleterious effect on the degree of order in the resulting pattern. Both, experiments and Cahn-Hilliard simulations suggest that during decompression the pattern suffers an order-order instability where the change in the lattice structure affects more profoundly short-range than long-range order. The lack of orientational order at small distances is due the presence of several kind of defects producing pattern instabilities. Appropriated control of the Sc conditions and the usage of thin film thickness allows to obtain patterns with long-range orientational order.

Acknowledgement

The authors are grateful with Consejo Nacional de Investigaciones Científicas y Técnicas and German Research Foundation, DFG.



Poster Presentation

Possibilities at the Polar beamline with APS-U and beyond

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In 2023 the upgrade of the Advanced Photon Source (APS-U) at Argonne National Laboratory to an MBA reverse bent lattice will be completed, delivering an extremely brilliant and highly coherent beam [1]. Polar, the beamline for polarization modulation spectroscopy at the APS sector 4, will leverage the upgraded source to push resonant scattering and spectroscopy experiments into new frontiers, with extreme sample environments, coherence-based techniques, and polarization control at the source. In this contribution, we will present details of the proposed Polar beamline as well as examples of new possibilities in the direction of resonant magnetic diffraction and XMCD experiments.

Fast x-ray polarization switching between left and right circular as well as between horizontal and vertical linear polarization will be possible with the new Superconducting Arbitrarily Polarizing Emitter (SCAPE) undulators, which are currently being designed for the POLAR beamline. Two experimental setups will make use of this new source and will allow diffraction (XRD, REXS, XRM) as well as absorption spectroscopy (XMCD, XMLD) experiments covering a wide range of absorption edges. The beamline will make accessible especially the energy range above 14 keV for magnetic spectroscopy experiments, normally not reachable at conventional hard-x-ray beamlines using phase plates for polarization manipulation and will enable investigation of magnetic properties of materials at the 5f L- and 4d K-edges using spectroscopic methods. Small focused and coherent beams down to 100 nm will allow reaching new areas in terms of resolution, by employing direct imaging or ptychographic [2] methods, at low temperature, high magnetic fields and high pressures. Beamline optics will be designed to reduce vibrations to guarantee small focus sizes.

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Acknowledgement

Work at Argonne is supported by the U.S. Department of Energy, Office of Science, under contract No. DE-AC-02-06CH11357.



Poster Presentation

Pressure and temperature effect on the structural properties of $\text{Mn}_{0.9}\text{Co}_{0.1}\text{NiGe}$ Heusler Alloy.

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Materials that present negative thermal expansion properties (NTE) have been studied due to the technological applicability that they can find and because it is a topic of high scientific interest aiming to better understanding the physical mechanisms responsible for the unusual properties of this class of materials. Recently studies has observed pronounced expansions in the structural lattice of some intermetallic compounds of the $\text{MM}'\text{X}$ family (where M and M'= transition metal and X = Si, Ge and Sn) when cooled [1]. Aiming to contribute with the study of the $\text{MM}'\text{X}$ compound structural stability, samples of the $\text{Mn}_{0.9}\text{Co}_{0.1}\text{NiGe}$ compound were synthesized by arc melting. X-ray diffraction measurements were performed, as a function of external parameters such as temperature and pressure and the obtained data were analyzed by using the Rietveld method. The results show that $\text{Mn}_{0.9}\text{Co}_{0.1}\text{NiGe}$ exhibits hexagonal Ni_2In -type structure at room temperature and as temperature decrease, a structural phase transition for TiNiSi - type orthorhombic structure is observed. External pressure induces the hexagonal phase at $T = 100$ K. The hexagonal phase fraction continuously increase with the increase of the applied pressure reaching $\sim 56.3\%$ for $P = 4.5$ GPa and 85.5% for $P = 12$ GPa, maximum applied pressure. As pressure increases, the distance between the nearest Mn atoms (D1), responsible for the magnetic ordering in the material significantly decreases ($\delta D1^{\text{orth}} \sim 2.23$ and $\delta D1^{\text{hex}} \sim 3.76$ in 12 GPa). The hexagonal phase fraction increase to 92.3% and negative thermal expansion effect is observed, when temperature increases from 100 to 160 K keeping the sample presses with 12 GPa. Deformed orthorhombic phase was observed when the pressed sample was cooled down from 160 K to $T=100$ K. The structural properties of the $\text{Mn}_{0.9}\text{Co}_{0.1}\text{NiGe}$ compound are strongly depending of the temperature and pressure external parameters.

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Acknowledgement

The authors would like to thank the financial support of the Brazilian agencies CNPq, CAPES, FAPEMA and also the LNLS (XDS station) staff.



Poster Presentation

Pressure-dependent Study of $\text{PbMn}_7\text{O}_{12}$ by Synchrotron X-ray powder diffraction

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The $\text{PbMn}_7\text{O}_{12}$ (PMO) belongs to the family of $\text{AMn}_7\text{O}_{12}$ quadruple perovskites whose members may present interesting multiferroic properties. The PMO is synthesized under high pressure (7.5 GPa) and high temperature (1373 K) conditions[1] and, similarly to $\text{CdMn}_7\text{O}_{12}$, $\text{SrMn}_7\text{O}_{12}$ and $\text{CaMn}_7\text{O}_{12}$ [2], crystallizes in the R-3 space group at room temperature. Temperature-dependent analyses of PMO [3] reveals that its multiferroic characteristics arise only in the long-range magnetic ordered phase which given to this material a spin-driven multiferroic characteristic. In addition, a structural phase transition from rhombohedral symmetry to a cubic (Im-3) symmetry given by charge ordering is reported at 397 K through temperature-dependent x-ray powder diffraction analysis. Nevertheless, no information about PMO structural behavior under pressure variation is reported until now. In this work we present the pressure dependent behavior analysis of PMO synthesized through high-pressure and high-temperature technique, by monitoring its lattice parameters behavior where were observed two possible phase transitions around 8.5 and 19 GPa. These Structural changes are similar to those observed for another quadruple perovskite $\text{CaMn}_7\text{O}_{12}$ [4]. The presented analyses were carried out through the synchrotron x-ray diffraction technique at the XDS beam line of National Laboratory of Synchrotron Light (LNLS) located at CNPEM.

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Acknowledgement

The Brazilian authors acknowledge the partial financial support from CNPq, CAPES, and FUNCAP Brazilian funding agencies.



Poster Presentation

Pressure studies on CaMn_2Bi_2 , a possible Mn-based hybridization gap semiconductor

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At ambient pressure and high temperatures, CaMn_2Bi_2 behaves as a single-band semimetal that orders antiferromagnetically below $T_N = 150$ K. At low temperatures, multi-band effects and a large magnetoresistance emerge along with an activated behavior typical of degenerate semiconductors [1,2]. The activation gap is estimated to be approximately 20 K. Band-structure calculations indicate that the activation gap is formed by the hybridization of one $3d^5$ Mn electron with the Bi p bands [1]. In fact, a Mn-pnictide hybridization was observed in ARPES experiments in similar compounds [3]. In this regard, applied pressure is an ideal tuning parameter by changing the orbital overlap and the Mn-pnictide hybridization without introducing disorder in the system. Therefore, we report electrical transport measurements on CaMn_2Bi_2 single crystals under applied pressure. Applied pressure favors both the antiferromagnetic order, at a rate of 0.40(2) K/kbar, and the activation gap by about 70% at 20 kbar. This gap enhancement is typical of correlated narrow-gap semiconductors such as FeSi and $\text{Ce}_3\text{Bi}_4\text{Pt}_3$ and places CaMn_2Bi_2 as a possible Mn-based hybridization-gap semiconductor.

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Poster Presentation

Spin rotation in Cd-doped Ce_2RhIn_8 induced by applied pressure

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In this work we present the pressure-dependent magnetic structure of $\text{Ce}_2\text{RhIn}_{7.79}\text{Cd}_{0.21}$ investigated by neutron magnetic diffraction (NMD) experiments. Through such techniques, it is possible to combine doping and applied pressure to tune the system's ground state (GS) considering that the moment's direction may be connected to the evolution of the crystalline electric field (CEF) effects. Cd-doped $\text{Ce}_m\text{M}_n\text{In}_{3m+2n}$ compounds exhibit fascinating electronic and magnetic behavior [1,2]. Particularly for Ce_2MIn_8 , Cd-doping favors magnetic states; for $M = \text{Rh}$ the Néel temperature (T_N) increases and long order magnetism for $M = \text{Ir}$ [3]. The NMD measurements were performed in the BT-9 triple axis neutron spectrometer at NCNR, with a designed aluminum pressure cell using gaseous He as transmitting medium. For $P < 6$ kbar there were no changes in the propagation vector $(1/2, 1/2, 0)$ nor T_N (4.8 K). As pressure increases, we observed changes in the moment's direction from 47° (at ambient pressure) towards the ab-plane at about 6 kbar. We have also measured electrical resistivity $\rho(T, P)$ to investigate how applied pressure tune T_N and the maximum of $\rho(T)$. The experiments were carried up to $P < 40$ kbar out with a clamp-type cell using Fluorinert as transmitting medium. To gain further insight into the role of CEF effects over the magnetic structure, we analyzed macroscopic data using a mean field model that accounts the tetragonal CEF. Preliminary results suggest that the evolution of the Ce^{3+} CEF scheme and GS wave-function can be affected by Cd-doping and pressure in order to explain the changes in the magnetic structure in these systems, modifying its orbital distribution in correlation to the appearance of magnetism or superconductive states.

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Poster Presentation

Stability of nitrogen expanded austenite under very high pressures

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Protective films and layers can effectively increase the lifespan of materials, by providing them protection against corrosion and abrasion even at elevated temperatures and mechanical stresses. There are extensive data demonstrating that the S-phase (expanded austenite) improves the surface mechanical properties of austenitic steels, which is also less susceptible to corrosion than the parent substrate. This phase, often produced by plasma-based nitriding [1,2], consists of a saturated nitrogen solid solution where the lattice experiences crystallographic orientation-dependent biaxial compressive stresses [3]. It is also metastable and is formed under non-thermodynamic equilibrium conditions. To evaluate the S-phase stability under additional internal stresses, we subjected grains of a plasma nitrided AISI 316L powder to extremely high pressures, ranging from atmospheric to ~30 GPa. The experiments were carried out with a Diamond Anvil Cell in the X-ray Diffraction and Spectroscopy (XDS) line of the Brazilian Synchrotron Light Laboratory. With pressure increments of ~1 GPa, X-ray transmission diffraction patterns were obtained under 10 min exposure time. The beam energy was 20 keV. The diffractograms were normalized based on the ring current for each of the measurements. The relative amount of the S-phase and austenite was inferred from the integrated intensities of the corresponding crystallographic planes. The S-phase contribution, evaluated through the (200) and (111) planes, significantly increased with pressure as a result of the nitrogen concentration change, which occurred mainly after the yield point. From the yield point on, entropy increased as a function of the density of defects, with the subsequent decrease of the Gibbs free energy. This led to a phenomenon observed for the first time in this work, the formation of stable nitrides existing only in a specific pressure range.

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Acknowledgement

The authors are grateful to the Brazilian Synchrotron Light Laboratory and CAPES that made this work possible.



Poster Presentation

Temperature and high pressure effects on the structural features of CeAl and NiAl catalytic oxides by Raman spectroscopy

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Several studies focus on the investigation of high pressure and temperature effects and how these factors can affect the catalytic performance of the oxides [1-4]. For instance, some catalytic measurements are carried out in wide range of temperatures ($30 < T < 700^{\circ}\text{C}$) and pressures ($0.1 < p < 16 \text{ GPa}$), which represent the typical values used in catalytic reactions for hydrocarbon transformations. Hence, a particular reaction condition can be designed through the spectroscopic investigations to be applied in a catalytic system, obtaining accurate measurements at extreme reaction conditions [5-7]. Then, the effects can be indirectly monitored to extend the capabilities of the oxides and achievement made with them in the reactions. In this study, high temperature and pressure effects on the physicochemical properties of CeAl and NiAl binary oxides catalysts were investigated. The CeAl and NiAl composites presented crystallographic stability at low temperatures however, undertake a phase transformation of $\text{NiO}/\text{Al}_2\text{O}_3$ into NiAl_2O_4 , mostly without any deformation in its structure with increasing the temperature. It was also inferred that the binary oxides are more stables in comparison with monoxides. High pressure on CeAl sample improved the stability with addition of Al_2O_3 in the CeO_2 lattice. The results then suggest a good stability of CeAl and NiAl composite catalysts at high pressure and low temperature and show how to prospect of tuning the catalysis for surface reactions entirely through *in situ* spectroscopic investigations means.

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Acknowledgement

The authors thank Funcap financial support for this research project (FUNCAP BPI 03/2018 BP3-0139-00055.04.00/18) and CAPES/FUNCAP (23038.008860/2013-92 and 23038.007964/2012-07).



Poster Presentation

The conformation of the N-terminal of the Prion Protein is important to direct its route of aggregation.

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The mechanism of cellular prion protein (PrPC) conversion into prion scrapie (PrPSc) is considered the most important factor in the development of prion diseases. Recent studies have concentrated efforts in understanding the importance of PrP N-terminal tail in this process. Several studies have shown that PrP conversion can be induced by interaction with phospholipids. Phosphatidic Acid (PA) vesicles interact with recombinant PrP (rPrP), leading to the formation of amorphous aggregates and amyloid fibrils, close to PrPSc structure. Our aim was to elucidate in which conditions PA may induce rPrP conversion into amyloid fibrils and to observe the PrP conformation that might favor this route of aggregation. We subjected the samples to different conditions (temperature and chaotropic agents) and used light scattering, circular dichroism, fluorescence spectroscopy and electron microscopy measurements to obtain structural and stability information. We observed that PA induces rPrP fibrillization under all the temperatures tested, but high temperatures decreased fibril formation. Fibril secondary structure was not affected by high temperatures, whereas the thioflavin T binding did, but return to room temperature restored fibril signal. Using acrylamide as fluorescent quencher agent, we observed that lower temperatures decreases tryptophan accessibility to solvent, and these residues appear to be more hidden in the fiber core. Our results suggest that changes over PrP dynamics and flexibility are important to follow a fibrillization pathway induced by PA. The quaternary structure of these fibrils seems to be sensible to high temperatures, although its secondary structure is stable, forming an intermediate capable of reorganizing into fibers. N-terminal conformation seems to be important to determine the route for this aggregation.



Poster Presentation

Tuning magnetic coercivity with external pressure in iron-rhenium based ferrimagnetic double perovskites

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We studied the effect of physical pressure on the electronic and magnetic properties of ferrimagnetic double perovskites $A_2\text{FeReO}_6$ ($A=\text{Ca}, \text{Ba}$) using Re $L_{2,3}$ edge x-ray absorption spectroscopy and powder diffraction measurements. Volume compression is shown to dramatically increase the magnetic coercivity (H_c) in polycrystalline samples of both compounds with $\Delta H_c/\Delta V \sim 150\text{-}200 \text{ Oe}/\text{\AA}^3$. A nearly eight-fold increase in H_c , from 0.2 T to 1.55 T, is obtained in $\text{Ba}_2\text{FeReO}_6$ at $P=29 \text{ GPa}$. While no signs of structural phase transitions are seen in either sample to $\sim 30 \text{ GPa}$, the structural data points to a pressure-driven increase in tetragonal distortion of ReO_6 octahedra. A sizable but pressure-independent Re orbital-to-spin magnetic moment ratio is observed, pointing to the critical role of spin-orbit interactions at Re sites. We present a j_{eff} description of the electronic structure that combines effects of crystal field and spin-orbit coupling on the Re $5d^2$ orbitals and use this description to provide insight into the pressure-induced enhancement of magnetic anisotropy.



Poster Presentation

X-ray absorption study of Yb valence state as a function of applied pressure in the intermetallic complex $\text{YbFe}_2\text{Zn}_{(20-x)}\text{Cd}_x$ ($x=0.0, 1.0, 1.3, 1.4$) compounds.

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The Heavy Fermion compound $\text{YbFe}_2\text{Zn}_{20}$ (Sommerfeld coefficient $\gamma=535 \text{ mJ.mol}^{-1} \cdot \text{K}^{-2}$), which crystallizes in the $\text{CeCr}_2\text{Al}_{20}$ -type structure with space group $Fd-3m$ (227), was doped with Cd atoms to study the physics of hybridized ions in crystal lattices. In this structure Yb and Fe atoms occupy the Wyckoff position 8a and 16d, respectively, while the Zn atoms occupy three different crystallographic sites (16c, 48f and 96g) [1][3]. The introduction of Cd disturbs the system and an increase of the lattice parameter is observed. A refinement of crystalline structure of $\text{YbFe}_2\text{Zn}_{20}$ and $\text{YbFe}_2\text{Zn}_{18.6}\text{Cd}_{1.4}$ using single crystal x-ray diffraction data was performed to determine which crystallographic site Cd atoms occupy. Our results of refinements show that Cd substitutes only those Zn atoms that occupy specifically the 16c crystallographic site. The observed changes in the physical properties as a function of Cd amount reported by Cabrera-Baez et. al, they suggested a possible valence shift of the Yb ions due to a negative chemical pressure that the Cd substitution represents[1]. So, to investigate the valence state of Yb ions we measured the x-ray absorption near the Yb L3-edge (XANES) as a function of Cd amount and as a function of temperature. For all these measurements, within the experimental limitation, the obtained Yb valence is $+2.84 \pm 0.04$ and no changes were observed as a function of Cd amount and as a function of temperature. On the other hand, previous measurements of electrical transport under pressure for $\text{YbFe}_2\text{Zn}_{20}$ indicate that a quantum critical point (QCP) may be present at $\sim 9.8 \text{ GPa}$ [2]. Inspired by this result, in the next step of this work we propose to measure the Yb L3-edge x-ray spectrum as a function of physical pressure to probe any possible valence shift of Yb ions near the proposed QCP.

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Acknowledgement

This work was supported by CAPES, CNPq, FAPESP 2017/10581-1, UNICAMP, IFGW Grupo de Materiais Quânticos - UFABC. We also want to thank the LNLS staff for the technical support.



Poster Presentation

X-ray diffraction with Synchrotron Radiation Study of the 2-(α -methylbenzylamino)-5-nitropyridine crystal at high pressure

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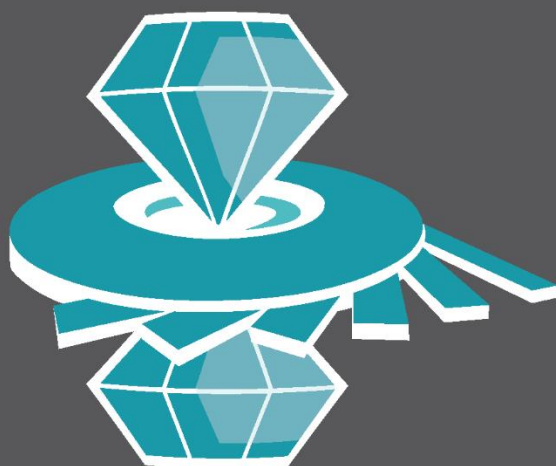
The conjugated 2-(α -methylbenzylamino)-5-nitropyridine crystalline system (MBAMP) present several important physical properties such as piezoelectricity, ferroelectricity and non-linear optical properties (NLO). It is a promising organic crystal due to their non-linear optical properties, being suitable for applications in optoelectronic such as optical modulation, frequency doubling and optical communication devices [1-6]. In this work, the effect of pressure on 2-(α -methylbenzylamino)-5-nitropyridine single crystal has been studied by X-ray powder diffraction up to 10 GPa. High-resolution X-ray powder diffraction measurements were performed at the X-ray Diffraction and Spectroscopy (XDS) station at Brazilian Synchrotron Light Laboratory, LNLS in Campinas, Brazil. X-rays diffraction experiments were carried out using a synchrotron radiation with 20 Kev, and an area detector. Changes in diffractions patterns confirms that that two changes in the molecular configuration takes place bellow 0.5 GPa, as observed by Raman spectroscopy. A possible explanation for these effects is that the changes in the monoclinic unit cell dimensions observed cause probably a rotational movement of the benzene ring (in the benzyl group) and neighboring CH₃ group around the N1-C9.

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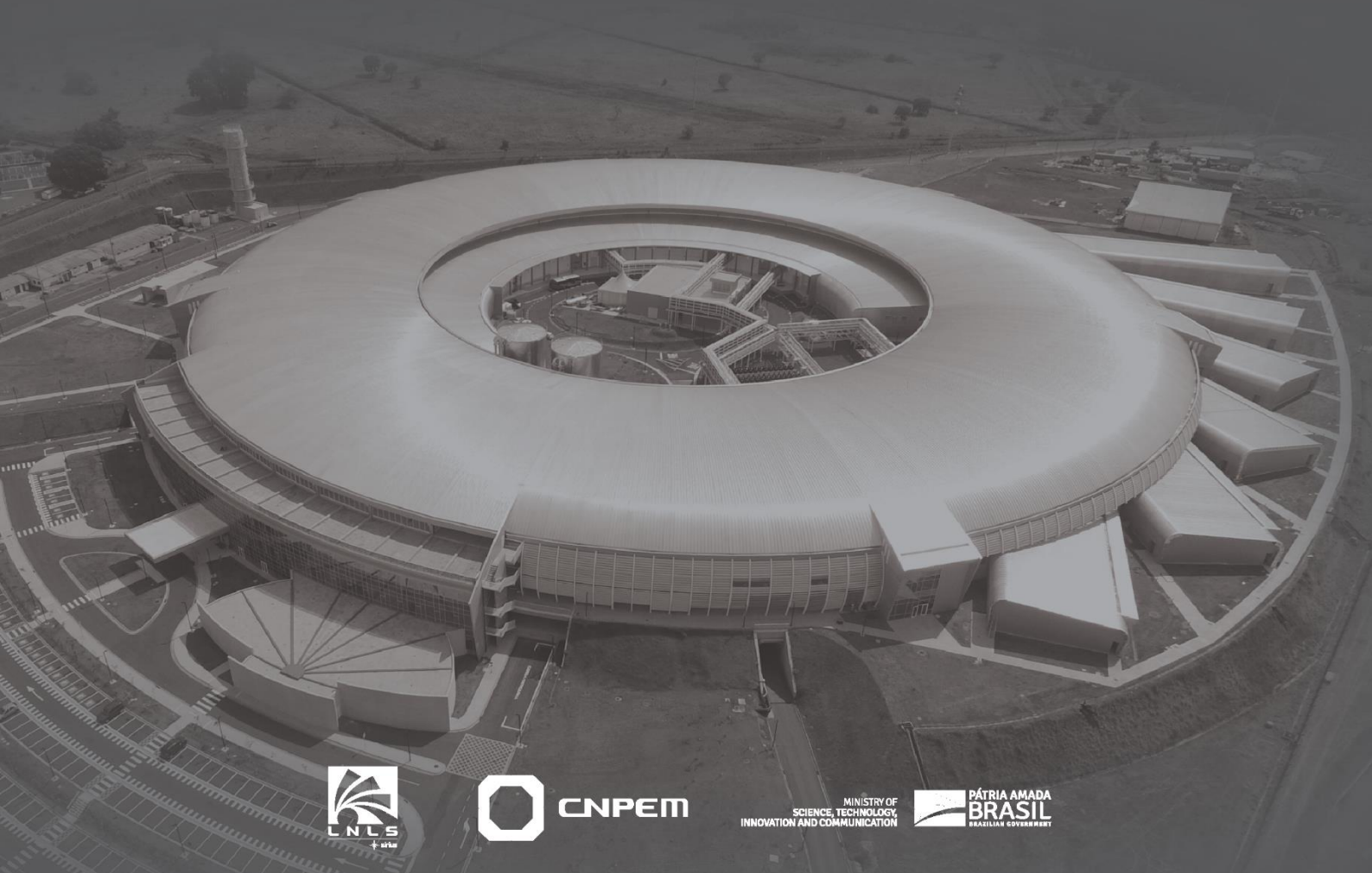
Acknowledgement

The authors acknowledge the financial support from the Brazilian agencies CNPq, CAPES and FAPEMA.



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INNOVATION AND COMMUNICATION

