

# 2015 IUCr High Pressure workshop – Campinas/SP/Brazil

## FINAL PROGRAM (including last minute changes)

### SATURDAY – 12 September 2015

|                              |  |
|------------------------------|--|
| <b>16:00</b><br><b>16:30</b> | Shuttle Buses from the Hotel to the LNLS Campus (please choose between the first or second bus time) |
| <b>17:00</b>                 | <b>Registration</b>  |
| <b>18:00</b>                 | <b>Get together reception at the LNLS/CNPEM campus</b>   |
| <b>20:00</b><br><b>20:30</b> | Shuttle bus back to the Hotel (please choose between the first or second bus time)                   |

### SUNDAY – 13 September 2015

|                              |  |   |
|------------------------------|--|---|
| <b>7:40</b><br><b>8:10</b>   | Shuttle Buses from the Hotel to the LNLS Campus (please choose between the first or second bus time) |   |
| <b>8:40</b>                  | <b>Opening remarks</b>   |   |
| 8:40 – 8:50                  | <b>Andrzej Katruziak</b><br>(IUCr HP Commission)   | Welcome and info about the IUCr HP Commission   |
| 8:50 – 9:10                  | <b>Narcizo Souza-Neto</b><br>(LNLS/SIRIUS)   | Welcome and info about LNLS and SIRIUS  |
| <b>9:10</b>                  | <b>High-pressure experiments and data deposition (Elena Boldyreva &amp; Nicholas Brooks)</b>         |   |
| 9:10 – 9:50                  | <b>K. Dziubek</b>  | “Deposition of high-pressure data and metadata”   |
| 9:50 – 10:30                 | <b>J. A. Lima Jr</b>   | “High pressure studies in crystalline amino acids”  |
| <b>10:30</b>                 | <b>Coffee Break</b>  |   |
| <b>11:00</b>                 | <b>Crystallographic controls on rheology and elasticity (Guoyin Shen &amp; Lowell Miyagi)</b>        |   |
| 11:00 – 11:40                | <b>L. Miyagi</b>   | “Synchrotron radial diffraction studies at high pressures and temperatures in the diamond anvil cell”   |
| 11:40 – 12:20                | <b>S. Hunt</b>   | “Deformation T-Cup: A 6-8 / Kawai-style deformation apparatus for controlled strain-rate deformation at pressures in excess of 20 GPa”                                |
| 12:20 – 13:00                | <b>H. Marquardt</b>  | “Internally consistent elasticity measurements of FIB-prepared single-crystals at high-pressure and high-temperature by Brillouin spectroscopy and X-ray diffraction” |
| <b>13:00</b>                 | <b>Lunch Break</b>   |   |
| <b>14:30</b>                 | <b>High-pressure chemistry, synthesis and biological systems (Boris Zakharov)</b>                    |   |
| 14:30 – 15:10                | <b>J. Haines</b>   | “Use of Fourier Maps to Study High Pressure Guest Insertion and Polymerization in Zeolites”   |
| 15:10 – 15:50                | <b>N. Brooks</b>   | “Probing membrane structure and dynamics at high pressure”  |
| 15:50 – 16:30                | <b>D. Paliwoda</b>   | “A new high-pressure phase of ferrocene”  |
| <b>16:30</b>                 | <b>Poster session (together with a Special Coffee Break)</b>   |   |
| <b>19:00</b><br><b>19:30</b> | Shuttle bus back to the Hotel (please choose between the first or second bus time)                   |   |

## Monday – 14 September 2015

**7:30**  
**8:00** Shuttle Buses from the Hotel to the LNLS Campus (please choose between the first or second bus time)

### **8:30 Computational approaches (Renata M. M. Wentzcovitch)**

|              |                        |   |
|--------------|------------------------|---|
| 8:30 – 9:10  | <b>R. Wentzcovitch</b> | “Spin crossover systems in the deep mantle”   |
| 9:10 – 9:50  | <b>K.-M. Ho</b>        | “Crystal Structure Predictions Using Adaptive Genetic Algorithm and Motif Search methods” |
| 9:50 – 10:30 | <b>K. Umemoto</b>      | “Volume isotope effects in ice under high pressure by first principles”                   |

**10:30 Coffee Break**

### **11:00 Materials Science (Julien Haines)**

|               |                      |  |
|---------------|----------------------|--|
| 11:00 – 11:40 | <b>V. Solozhenko</b> | “Boron-phosphorus system at high pressure”   |
| 11:40 – 12:20 | <b>A. Cairns</b>     | “Pushing the limits: designing next-generation negative compressibility materials” |
| 12:20 – 13:00 | <b>S. Deemyard</b>   | “Structures of lithium isotopes at low temperature”                                |

**13:00 Lunch Break**

### **14:30 Polymorphism and crystal chemistry (Ania Olejniczak)**

|               |                    |  |
|---------------|--------------------|--|
| 14:30 – 15:10 | <b>M. Pravica</b>  | “Novel fluorine chemistry under extreme conditions using useful hard x-ray photochemistry” |
| 15:10 – 15:50 | <b>M. Probert</b>  | “Routes to More Polymorphs and Phase Changes”  |
| 15:50 – 16:30 | <b>R. Miletich</b> | “Decoding the mechanisms and pathways of pressure-driven structural transitions”           |

**16:30 Coffee Break**

### **17:00 High-pressure crystallography in earth and planetary science (Simon Redfern & Rommulo Conceicao)**

|               |                     |  |
|---------------|---------------------|--|
| 17:00 – 17:40 | <b>Y. Le Godec</b>  | “Next generation synchrotron portable Large Volume High-P/T/Stress/Tomography Cell for Extreme Chemistry and Earth Sciences” |
| 17:40 – 18:20 | <b>S. Redfern</b>   | “New challenges and opportunities for mineral physics of the deep Earth”   |
| 18:20 – 19:00 | <b>R. Conceicao</b> | “The role of clay minerals on the volatiles transport to the mantle and internal heating of the Earth”                       |

**19:00** Shuttle transfer to the restaurant

**19:20 Workshop Dinner (at a Brazilian Churrascaria)**

**21:30** Shuttle transfer to the hotel and guest house

## Tuesday – 15 September 2015

|               |   |  |  |
|---------------|---|--|--|
| <b>7:30</b>   | First shuttle Bus from the Hotel to the LNLS Campus (IF PLANNING TO VISIT THE SIRIUS SITE)                      |  |  |
| <b>8:00</b>   | Second shuttle Bus from the Hotel to the LNLS Campus (for those not planning to visit Sirius construction site) |  |  |
| 8:00 – 9:00   | <b>VISIT TO SIRIUS CONSTRUCTION SITE</b>  |  |  |
| <b>9:10</b>   | <b>New Frontiers in Extreme Conditions Crystallography (Haozhe Liu)</b>   |  |  |
| 9:10 – 9:50   | <b>M. Zaworotko</b>   | “High pressure applications of porous metal-organic materials”   |  |
| 9:50 – 10:30  | <b>J. Smith</b>   | “Fast compression/decompression of materials in diamond anvil cells”   |  |
| <b>10:30</b>  | <b>Coffee Break</b>   |  |  |
| <b>11:00</b>  | <b>High-pressure spectroscopy (João A. H. da Jornada &amp; Kamil Dziubek)</b>                                   |  |  |
| 11:00 – 11:40 | <b>R. Bini</b>  | “Pressure induced reactivity in molecular crystals: accessing the dynamics at molecular level by complementary structural and spectroscopic experiments” |  |
| 11:40 – 12:20 | <b>C. Murli</b>   | “Hydrogen Bonded Organic Molecular Solids under Pressure”  |  |
| 12:20 – 13:00 | <b>A. Gomes</b>   | “Resonance high-pressure Raman spectroscopy in nanocarbon materials”   |  |
| <b>13:00</b>  | <b>Lunch Break</b>  |  |  |
| <b>14:30</b>  | <b>Rising Stars (Andrzej Katrusiak &amp; Simon Clark)</b>   |  |  |
| 14:30 – 15:10 | <b>G. Finkelstein</b>   | “Magnesiowüstite at high pressure using single-crystal synchrotron methods”  |  |
| 15:10 – 15:50 | <b>M. Marcondes</b>   | “Hybrid experimental/theoretical thermodynamics and thermoelasticity of materials: the high T NaCl pressure scale”                                       |  |
| 15:50 – 16:30 | <b>O. Kurakevych</b>  | “New silicon and carbon materials by in situ high pressure synthesis”  |  |
| <b>16:30</b>  | <b>Closing Remarks</b>  |  |  |
| <b>18:00</b>  | Shuttle transfer to the hotel   |  |  |

A tour around the synchrotron should be fitted in the slots during the workshop.