PAUL SCHERRER INSTITUT

PSD Mini Symposium

Polymerization, metal transition and multiferroics

Tuesday, April 9, 2019

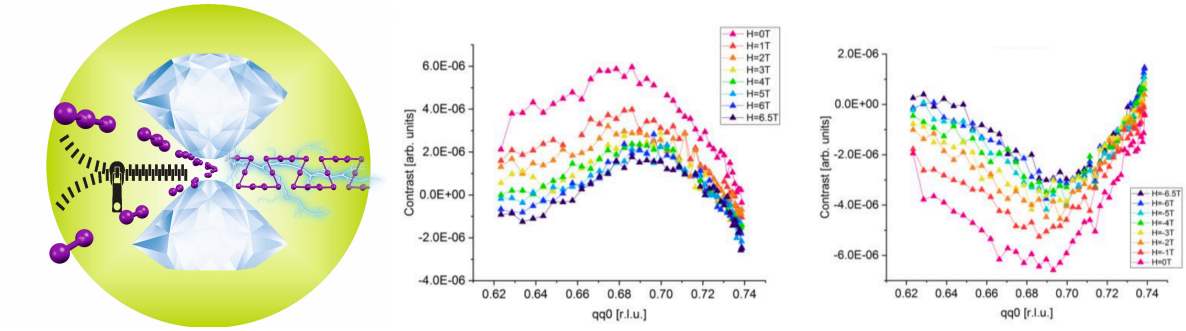
10:00 to 11:45, WBGB 019

10:00 Pressure-induced Polymerization and Electrical Conductivity of a Polyiodide
Tomasz Poręba, M. Ernst, N. Casati and P. Macchi

10:30 Orbital dynamics during an ultrafast insulator to metal transition
Sergii Parchenko, E. Paris, D. McNelly, E. Abreu, M. Dantz, E. M. Bothschafter, W. F. Schlotter, M-F Lin, S. F. Wandel, G. Coslovich, S. Zohar, A. H. Reid, G. L. Dakovski, C. Saathe, M. Agaaker, J. E. Nordgreen, S. L. Johnson, T. Schmitt, and U. Staub

11:00 Coffee break

11:15 Study on type II multiferroics under high magnetic and electric field
Nazaret Ortiz-Hernandez, S. Parchenko, J. R. Linares Mardegan, Y. W. Windsor, E. Schierle, E. Weschke, J. A. Huever, B. Noheda, C. Schneider, G. Nisbet and U. Staub



Pressure-induced Polymerization and Electrical Conductivity of a Polyiodide

Tomasz Poręba†‡, Michelle Ernst†, Nicola Casati‡, Piero Macchi†

† Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3,Bern, Switzerland
‡ Laboratory for Synchrotron Radiation, Paul Scherrer Institute, 5232 Villigen – PSI, Switzerland

We reported the high-pressure structural characterization of an organic polyiodide salt in which a progressive addition of iodine to triiodide groups occurs. Compression leads to the initial formation of discrete heptaiodide units, followed by polymerization to a 3D anionic network. Although the structural changes appear to be continuous, the insulating salt becomes a semiconducting polymer above 10 GPa. The features of the pre-reactive state and the polymerized state are revealed by analysis of the computed electron and energy densities. The unusually high electrical conductivity can be explained with the formation of new bonds.

[1] Poreba, T. et al. (2019), Angew. Chem. Int. Ed.

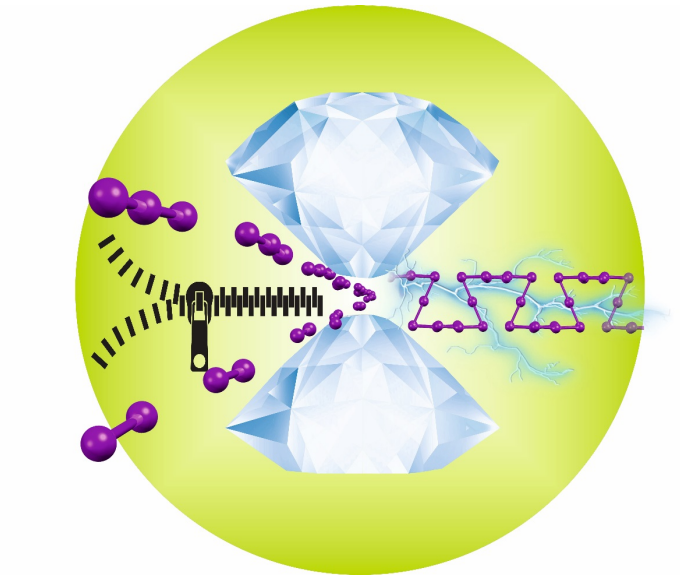


Figure 1. High-pressure, as a "zipper", forces I_3^- and I_2 units to form the conductive polymeric chain.

Orbital dynamics during an ultrafast insulator to metal transition

Sergii Parchenko[1], Eugenio Paris[1], Daniel McNelly[1], Elsa Abreu[2], Markus Dantz[1], Elisabeth M. Bothschafter[1], William F. Schlotter[3], Ming-Fu Lin[3], Scott F. Wandel[3], Giacomo Coslovich[3], Sioan Zohar[3], Alexander H. Reid[3], Georgi L. Dakovski[3], Conny Saathe[4], Marcus Agaaker[5], Joseph E. Nordgreen[5], Steve L. Johnson[2], Thorsten Schmitt[1], and Urs Staub[1]

[1] Swiss Light Source, Paul Scherrer Institute, CH-5232 Villigen PSI, Switzerland

[2] Institute for Quantum Electronics, ETH Zürich, 8093 Zürich, Switzerland

[3] LCLS, Stanford National Accelerator Laboratory (SLAC), Menlo Park, California 94025, USA

[4] Lund University, MAX Lab 4, Box 118, SE-22100 Lund, Sweden

[5] Uppsala University, Department of Physics & Astronomy, S-75120 Uppsala, Sweden

e-mail: sergii.parchenko@psi.ch

Recent achievements in developing of bright and ultrashort X-ray pulses open new possibilities to use X-rays as a probe in experiments on ultrafast time scale. We aimed to study laser induced insulator to metal transition with Resonant Inelastic X-ray Scattering (RIXS) in soft X-ray regime to track directly the changes in orbital states on the ultrafast time scale. The investigating material was thin film of V_2O_3 – prototypical Mott Hubbard material which have insulator to metal transition at T=160K. We pump it with 800nm p-polarized fs laser pulse to induce the transition. The experiment was made at LCLS free electron laser. During the experiment, we successfully excite the insulator to metal transition and collect RIXS spectra for different delay times to follow the transition. Obtained spectra are in good agreement with data, collected in static regime using synchrotrons. With this study we want not only to prove possibility of making ultrafast RIXS experiments but also to clarify electron-phonon coupling in such a strongly correlated system. Obtained results have significant importance both for instrumentation development and deeper understanding of electron band structure dynamics and its relation to the crystal structure.

Study on type II multiferroics under high magnetic and electric field

N. Ortiz-Hernandez[1], S. Parchenko[1], J. R. Linares Mardegan[2], Y. W. Windsor[3], E. Schierle[4], E. Weschke[4], J. A. Huever[5], B. Noheda[5], C. Schneider[1], G. Nisbet[6], U. Staub[1]

1 Swiss Light Source, Paul Scherrer Institute, 5232 Villigen, Switzerland.
2 Deutsches Elektronen-Synchrotron, 22607 Hamburg, Germany.
3 Fritz-Haber-Institut der Max-Planck Gesellschaft, 14195 Berlin, Germany.
4 Helmholtz-Zenturm Berlin fur Materialien und Energie GmbH, Albert-Einstein-Strasse 15, 12489 Berlin, Germany.
5 Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands.
6 Diamond Light Source Ltd. OX11 0DE Didcot, United Kingdom.

Type II multiferroic materials have attracted a lot of attention due to the strong coupling between ferroelectric and magnetic order parameter they exhibit, giving the possibility of controlling magnetic properties by applying electric field or vice versa.
We present two different studies on two different type II multiferroics:

1. **$CoCr_2O_4$** (CCO) is a type II multiferroic material and in addition presents a remnant magnetic moment (ferrimagnet) which is not common in type II multiferroics.
   Here we present resonant soft x-ray diffraction in high magnetic fields on epitaxially grown CCO, where we find a direct correlation between magnetic fields and cycloidal rotation direction that is expected determine the induced polarization direction.

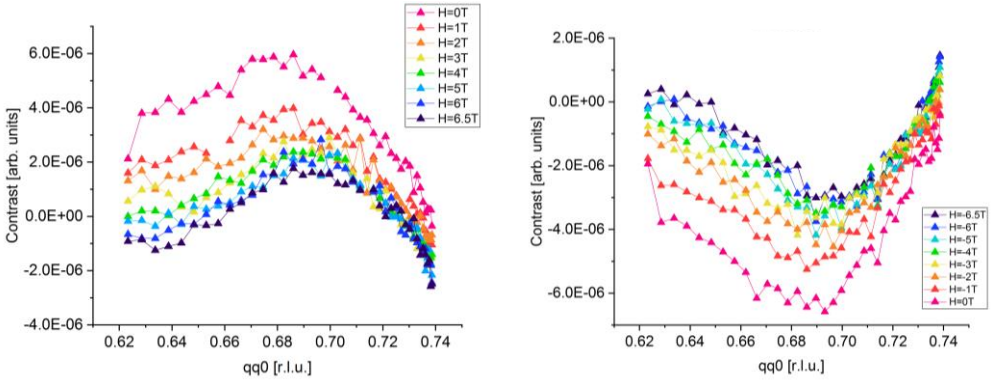


Figure 1.CCO data of the intensity contrast (C+ - C-) in function of the propagation vector qq0 for different magnetic fields.

2. The orthorhombic (Pbnm) **$HoMnO_3$** is of particular interest due to its high magnetically-induced polarization values (*P*) and magnetoelectric coupling strength. The mechanism behind this involves symmetric exchange striction. We investigated the atomic distortion to identify the broken symmetry of Pbnm in thin films of $HoMnO_3$ at low temperature. Forbidden reflections for Pbnm has been observed showing the structural phase transition. Moreover, we present direct measurements of the polar distortion visualized by the difference diffraction intensity from opposite domains.

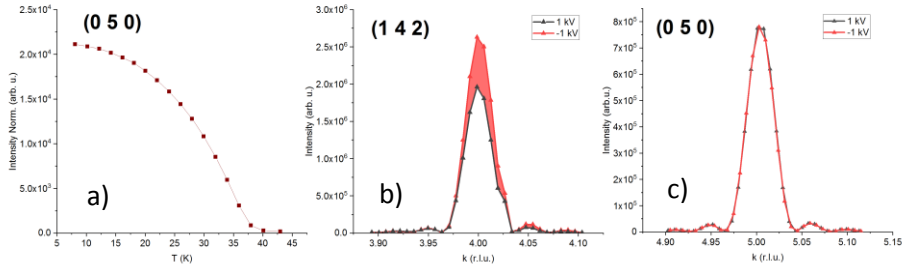


Figure 2. $HoMnO_3$ data. (a) Temperature dependence of (050) forbidden reflection for Pbnm symmetry. (b-c) k-scans of 2 reflection for 2 opposite E-fields (voltage applied: + 1 kV and -1 kV).