Contribution ID: **121** Type: **Poster**

Nuclear resonance scattering polarimetry on single crystals of iron spin crossover compounds

Monday, 17 September 2018 17:45 (15 minutes)

The combination of nuclear forward scattering as time-domain synchrotron-based nuclear resonant scattering method with high-purity polarimetry is a novel approach to probe electronic anisotropies in metal-containing compounds ranging from biological molecules to solid state systems.
This method is based on exploring the polarization dependence of the nuclear hyperfine transitions at the 14.4 keV nuclear resonance of ⁵⁷Fe. The use of a crossed polarizer-analyzer setup [1] allows the suppression of the incident σ-polarized non-resonant photons. Probing thereby single crystals, the magnitude and orientation of the electric field gradient (EFG) at the Mössbauer nucleus produced by charge anisotropies is deliverable.
The application of this method is shown by means of the study of the monoclinic phase of the spin crossover (SCO) complex [Fe(PM-BiA)₂(NCS)₂] (**1**). Iron(II) SCO compounds can be switched reversibly from the low spin to the high spin state, e.g. by variation of temperature [2]. The presence of a strong EFG at the Mössbauer nucleus that leads to a pure electric hyperfine interaction was shown by density functional theory calculations and conventional Mössbauer experiments on a powder sample of **1**. The realised nuclear resonance scattering polarimetry experiments on a single crystal of **1** have delivered information in terms of magnitude and orientation of the EFG.
[1] B. Marx et al., Phys. Rev. Letters 110, 254801 (2013)
[2] P. Gütlich et al., Angew. Chem. 106, 2109 (1994)

Primary author: Mrs SCHERTHAN, Lena (Department of Physics, Technische Universitaet Kaiserslautern)

Co-authors: Dr WOLNY, Juliusz A. (Department of Physics, Technische Universitaet Kaiserslautern); Dr ISABELLE, Faus (Department of Physics, Technische Universitaet Kaiserslautern); Dr LEUPOLD, Olaf (Deutsches Elektronen-Synchrotron DESY); Dr SCHULZE, Kai S. (Helmholtz-Institut Jena; Institute of Optics and Quantum Electronics); Dr HOEFER, Sebastian (Helmholtz-Institut Jena; Institute of Optics and Quantum Electronics); Dr LOETZSCH, Robert (Helmholtz-Institut Jena; Institute of Optics and Quantum Electronics); Dr MARX--GLOWNA, Berit (Helmholtz-Institut Jena; Institute of Optics and Quantum Electronics); Dr ANSON, Christopher E. (Institute of Inorganic Chemistry, Karlsruhe Institute of Technology); Prof. POWELL, Annie K. (Institut fuer Nanotechnologie; Institute of Inorganic Chemistry, Karlsruher Institut fuer Technologie); Dr USCHMANN, Ingo (Helmholtz-Institut Jena; Institute of Optics and Quantum Electronics); Dr WILLE, Hans-Christian (Deutsches Elektronen-Synchrotron DESY); Prof. PAULUS, Gerhard (Helmholtz-Institut Jena; Institute of Optics and Quantum Electronics); Prof. SCHUENEMANN, Volker (Department of Physics, Technische Universitaet Kaiserslautern); Prof. ROEHLSBERGER, Ralf (Deutsches Elektronen-Synchrotron DESY)

Presenter: Mrs SCHERTHAN, Lena (Department of Physics, Technische Universitaet Kaiserslautern)

Session Classification: Poster session 1

Track Classification: P1 Instrumentation and methods