

## MM 62: Topical Session (Symposium MM): Big Data in Materials Science - Managing and exploiting the raw material of the 21st century

Big Data VII

Time: Friday 11:15–12:45

Location: H 0107

**Topical Talk** MM 62.1 (27) Fri 11:15 H 0107

**Higher-dimensional synchrotron-based tomography for nanostructure characterization** — ●MANUEL GUIZAR-SICAÏROS — Paul Scherrer Institut, Villigen PSI, Switzerland

High-energy X-rays can probe the nanostructure of a broad range of biological and synthetic materials, based on electron-density heterogeneity. Currently, the high photon flux employed to carry out synchrotron experiments has increased the acquisition speed in measurements and enabled multidimensional characterization of materials. Alongside from direct structure imaging via tomography, scanning small-angle X-ray scattering (sSAXS) can be used to gather statistical information about the local nanostructure, in the range from 1 to 100 nm, on macroscopic samples of a few millimeters in size. Thus, sSAXS is very well suited to study correlation between heterogeneous nanostructure and macroscopic sample characteristics.

After a brief introduction I will describe our efforts towards automatic classification and segmentation of the large volumes of data generated by sSAXS and some of its applications. Furthermore I will discuss the combination of sSAXS with computed tomography, a technique we term small-angle-scattering tensor tomography (SASTT), which allows probing 3D nanostructure anisotropy, within subvolumes (voxels) of a sample. Some emphasis will be given on the measurement and algorithms used for reconstruction of the 6D spatially-resolved reciprocal-space map.

MM 62.2 (43) Fri 11:45 H 0107

**40 years of material science at ISOLDE-CERN using TD-PAC and MS** — ●JULIANA SCHELL<sup>1,2</sup>, PETER SCHAAP<sup>3</sup>, HANS-CHRISTIAN HOFSSÄSS<sup>4</sup>, and DORU C. LUPASCU<sup>2</sup> — <sup>1</sup>European Organization for Nuclear Research (CERN), Switzerland — <sup>2</sup>University of Duisburg-Essen, Germany — <sup>3</sup>TU Ilmenau, Germany — <sup>4</sup>Georg-August-Universität Göttingen, Germany

Since the late 70ies researchers at ISOLDE-CERN have been applying nuclear techniques to materials science research. A considerable infrastructure has been built up on-site to allow scientists to perform experiments using short-lived isotopes, especially using Time Differential Perturbed Angular Correlations (TDPAC) [1] and Mössbauer Spectroscopy (MS) [2, 3]. The online production of radioactive isotopes with high yield and elemental and isotopic purity allow the choice of the adequate probe to study the relevant solid state problem. In this context, TDPAC and emission MS are very powerful to characterize new materials and particularly atomic defects in them with very small concentrations of nuclear probes. Our facilities at ISOLDE-CERN are the world reference for these measurements. They are dedicated to many different purposes e.g. investigations of semiconductors oxides, photocatalytic materials, multiferroics, superconductors, metals, and alloys. In this presentation, we explore the multiple measurement possibilities.

References [1] J. Schell, P. Schaaf, and D. C. Lupascu, AIP Advances 7, 105017 (2017). [2] J. Schell, P. Schaaf et al. Not yet published. [3] MS Collaboration at ISOLDE-CERN: <http://e-ms.web.cern.ch/>

MM 62.3 (379) Fri 12:00 H 0107

**New Tolerance Factor to Predict Perovskite Oxide and Halide Stability** — ●CHRISTOPHER J. BARTEL<sup>1</sup>, CHRISTOPHER SUTTON<sup>2</sup>, BRYAN R. GOLDSMITH<sup>3</sup>, RUNHAI OUYANG<sup>2</sup>, CHARLES B. MUSGRAVE<sup>1</sup>, LUCA M. GHIRINGHELLI<sup>2</sup>, and MATTHIAS SCHEFFLER<sup>2</sup> — <sup>1</sup>University of Colorado Boulder, Boulder, USA — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — <sup>3</sup>University of Michigan, Ann Arbor, USA

Using the novel data analytics approach sure independence screening and sparsifying operator (SISSO) [1] an accurate one-dimensional tolerance factor ( $\tau$ ) is developed that correctly classifies 92% of compounds as perovskite or nonperovskite for an experimental dataset containing 576 ABX<sub>3</sub> materials. Importantly,  $\tau$  has nearly a uniform performance

across the five anion subsets: oxides (92%), fluorides (92%), chlorides (90%), bromides (93%), iodides (91%). In comparison, the widely used Goldschmidt tolerance factor ( $t$ ) achieves a maximum accuracy of only 74% for the same set of materials, with a significantly lower accuracy for chlorides (52%), bromides (56%), and iodides (33%) than for oxides (83%) and fluorides (85%). The accuracy of  $\tau$  combined with its simplicity, a continuous function of only the oxidation state of the A-site cation and Shannon ionic radii, allows for new physical insights into the stability of the perovskite structure and the prediction of more than 1,000 new stable inorganic and hybrid organic-inorganic double perovskite halides. [1] R. Ouyang, et al., arXiv:171003319 (2017).

MM 62.4 (163) Fri 12:15 H 0107

**Taming the Configurational Explosion - Statistical Learning for Structure Search** — ●LUKAS HÖRMANN, MICHAEL SCHERBELA, and OLIVER T. HOFMANN — Institute of Solid State Physics, Graz University of Technology, Austria

Monolayers of organic molecules on inorganic substrates often show rich polymorphism with diverse structures in differently shaped unit cells. Determining the different commensurate structures from first principles is far from trivial due to the large number of possible polymorphs. We pursue the SAMPLE approach[1][2], which is based on coarse-graining the potential energy surface and applying Gaussian Process Regression to efficiently find the energy of all polymorphs. To that end, we first determine adsorption geometries of isolated molecules as well as all possible unique substrate supercells. Then we combine each adsorption geometry with every super cell to generate all configurations. For a subset of these configurations, adsorption energies are determined using DFT. This subset serves as training data for the machine learning algorithm, that allows us to predict the adsorption energies for all polymorphs. Finally, all configurations with an adsorption energy below predefined energy threshold are reranked using DFT.

We demonstrate the capability of our approach for Naphtalene on Cu(111). We determine the adsorption energies for a large number of polymorphs and compare the results to the experimentally obtained phase diagram.

[1] Obersteiner, Hörmann, et. al., Nano Lett. 17 (7), pp 4453-4460

[2] Scherbela, Hörmann et. al., arXiv: 1709.05417

MM 62.5 (41) Fri 12:30 H 0107

**Machine learning the structure-energy-property landscapes of molecular crystals** — ●FELIX MUSIL<sup>1</sup>, SANDIP DE<sup>1</sup>, JACK YANG<sup>2</sup>, JOSHUA CAMPBELL<sup>2</sup>, GRAEME DAY<sup>2</sup>, and MICHELE CERIOTTI<sup>1</sup> — <sup>1</sup>COSMO, EPFL, Lausanne, Switzerland — <sup>2</sup>University of Southampton, Southampton, UK

Molecular crystals play an important role in several field of science and technology. They often crystallize in many different polymorphs with substantially different physical properties. To help prioritize the synthesis of candidate materials, atomic-scale modelling can be used to enumerate the stable polymorphs and to predict their properties, as well as to propose heuristic rules to rationalize the correlations between crystal structure and materials properties.

Here we show how a recently-developed machine-learning (ML) framework [1] can be used to achieve inexpensive and accurate predictions of the stability and properties of polymorphs, and a data-driven classification that is less biased and more flexible than typical heuristic rules. We discuss, as examples, the lattice energy landscapes and the automatic structural classification of pentacene and two azapentacene isomers that are of interest as organic semiconductor materials. We show that we can estimate lattice energies with sub-kJ/mol accuracy, using only a few hundred reference configurations, and provide a more detailed picture of molecular packing than that provided by conventional heuristics.

[1] De, S., Bartok, A. P., Csanyi, G., & Ceriotti, M. (2016). Phys. Chem. Chem. Phys., 18(20), 13754.