MM 63: Computational Materials Modelling - Electronic Structure of Complex Materials

Time: Thursday 17:30–19:00 Location: IFW A

MM 63.1 Thu 17:30 IFW A

Multistep stochastic mechanism polarization switching model — •Ruben Khachaturyan[1], Ankit Biswas[1], Anna Grünebohm[1], and Yuri Genenko[2] — [1]Interdisciplinary Center for Advanced Materials Simulation, Ruhr-Universität Bochum — [2]Institute of Materials Science, Technische Universität Darmstadt

The multistep stochastic mechanism (MSM) polarization switching model is a recent extension of the classical Kolmogorov-Avrami-Ishibashi model. It provides an easy way to describe polarization and strain kinetics of ferroelectrics with tetragonal symmetry. The model is now extended to rhombohedral and orthorhombic symmetries. The extended model can well fit experimental results, which evidence its capability to treat different symmetries. We try to utilize a machine learning algorithm based on linear regression to apply the modified MSM model to a system with a rhombohedral symmetry to get the best possible fitting of the experimental data. [1] **Stochastic multistep polarization switching in ferroelectrics**, Y.A. Genenko, R. Khachaturyan, J. Schultheiß, A. Ossipov, J. E. Daniels, and J. Koruza, **97(14)**, 144101 (2018)

MM 63.2 Thu 17:45 IFW A

First-principles investigation of the electromechanical response properties of ferroelectric HfO2 — •Sangita Dutta[1,2] and Jorge Iniguez[1,2] — [1]Luxembourg Institute of Science and Technology, Luxembourg — [2]University of Luxembourg, Luxembourg

Over the past few years, hafnia (HfO2) has been attracting attention due to its newly discovered ferroelectric behaviour [1]. This compound is a promising candidate for a variety applications ranging from ferroelectric memories to energy storage [2]. Interestingly, we note that, in spite of the very intense research focus on hafnia, a detailed understanding of response properties of ferroelectric hafnia is still missing in literature. In this present study, we compute the dielectric and piezoelectric responses of hafnia using first-principles density functional theory. More specifically, we work with the usual ferroelectric phase of hafnia (space group Pca21), and also investigate the variation of the electromechanical responses as a function of substitutional isovalent doping (i.e., Si, C, and other species replacing Hf atoms). In this talk, I will discuss our results and their implications for the optimization of the intrinsic response properties of ferroelectric hafnia.

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[1] T. S. Böscke, J. Muller, D. Bräuhaus, U. Schröder and U. Böttger.App. Phys. Lett. 99 (2011) [2] J. Muller, P. Polakowski, S. Muller and T. Mikolajick, ECS J.Solid State Sci.Technol. 4, N30-N35 (2015)

MM 63.3 Thu 18:00 IFW A

The Quantum Rectification Tensor of Three-Dimensional Materials — •Urmimala Dey[1,3], Oles Matsyshyn[1], Yan Sun[2], and Inti Sodemann[1] — [1]Max Planck Institute for the Physics of Complex Systems, Dresden 01187, Germany — [2]Max Planck Institute for Chemical Physics of Solids, Dresden 01187, Germany — [3]Indian Institute of Technology Kharagpur, Kharagpur 721302, India

We report on the first realistic calculations of the Quantum Rectification Tensor (QRT) of three-dimensional materials without inversion symmetry for the Weyl semimetal TaAs and the ferroelectric insulator LiAsSe2. The QRT is a fundamental property of any material without inversion symmetry which is dictated entirely by its Berry phase geometry, and it is determined by the Quantum Rectification Sum Rule that contains the Berry Curvature Dipole but also additional interband optical shift current contributions. In three dimensions the QRT is dimensionless when measured in fundamental constants of nature, namely, in units of the quantum of conductance divided by the quantum of flux. We will discuss the importance of this QRT as a figure of merit in the search for technologically promising bulk photovoltaic materials.

MM 63.4 Thu 18:15 IFW A

computational screening for anderson insulators — •yazhi xu[1], xudong wang[2], riccardo mazzarello[1], and wei zhang[2] — [1]RWTH Aachen University, Aachen, Germany — [2]Xi'an Jiaotong University, Xi'an, China

Anderson insulators are characterized by charge localization induced by crystal disorder. Recently, it was shown that the compound Ge1Sb2Te4 can crystallize into a metastable rocksalt-like structure that exhibits an Anderson insulating phase stemming from vacancy disorder. Furthermore, an insulator-metal transition can be triggered in these compounds by thermal annealing, which leads to vacancy ordering. Here, we perform a systematic computational screening for Anderson insulators in IV1V2VI4 compounds based on density functional theory. We consider the rocksalt-like phase and carry out geometry optimization and bonding analysis to determine their stability. For the stable models, we determine the localization of the electronic states relevant to transport.

MM 63.5 Thu 18:30 IFW A

Addressing the conflict of locating solvated electrons in alkali metal doped zeolites — •Debalaya Sarker[1,2], Sergey V. Levchenko[1,2], and Matthias Scheffler[2] — [1]Skolkovo Institute of Science and Technology, Moscow, RU — [2]Fritz-Haber-Institut der MPG, Berlin, DE

Doping faujasite Y (FAU-Y), a nanoporous aluminosilicate zeolite, with alkali metal atoms M (Na, K, Cs, etc.) is a promising way to produce outstanding basic catalysts. The dopants, along with extraframework metal atoms, often form M_4^{+3} clusters inside zeolite pores: leaving the valence electron of the dopant solvated and available for catalysis. Despite extensive experimental efforts, the distribution of the dopants and solvated electrons remains debated till date [1,2]. Combining a cluster expansion model, parameterized with extensive PBE+vdW calculations, and *ab initio* atomistic thermodynamics, we address this issue. Further, the electronic structure is calculated with hybrid HSE06 functional for low-energy configurations. We find that at temperatures >850 K Na atoms in NaY zeolites with two extraframework atoms per unit cell on average redistribute so that areas with lower and higher local concentrations emerge. The redistribution is driven by increased configurational disorder at both higher and lower concentrations. This explains why solvated electrons can be located inside both small and large cages in NaY, reconciling experiments assigning the solvated electrons to a particular pore type.

[1] A. R. Armstrong *et al.*, J. Am. Chem. Soc. **117**, 9087 (1995).
[2] W. Louisfrema *et al.*, Molecular Simulation **41**, 1371 (2015).

MM 63.6 Thu 18:45 IFW A

Comprehensive scan for nonmagnetic Weyl semimetals — •Qiunan Xu[1], Yang Zhang[1], Klaus Koepernik[2], Wujun Zhang[3], Jeroen van den Brink[2], Claudia Felser[1,4], and Yan Sun[1] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany — [3]School of Physical Science and Technology, ShanghaiTech University, Shanghai 200031, China — [4]Center for Nanoscale Systems,Faculty of Arts and Sciences, Harvard University,11 Oxford Street, LISE 308 Cambridge, MA 02138, USA

As the development of topological band theory, comprehensive databases about time reversal and crystalline symmetries protected nonmagnetic topological materials were developed via first-principles calculations recently. However, owing to the low symmetry requirement of Weyl points, the WSMs with Weyl points in arbitrary positions are still absent in the well-known databases. In this work, we develop an efficient algorithm to establish a database of nonmagnetic WSMs with Weyl points near Fermi level based on the total experimental noncentrosymmetric crystal structures in ICSD. Totally 49 Weyl semimetals were discovered to have nearly clean Fermi surface and Weyl points near Fermi level within 300 meV, and 12 of them are chiral structures hosting the quantized circular photogalvanic effect. In addition, the nonlinear optical response is studied and giant shift current is explored in the end. Besides nonmagnetic WSMs, our powerful tools can also be used in the discovery of magnetic topological materials.