

KFM 8: Crystal Structure / Real Structure / Microstructure

Chairman: Jan Schultheiß (NTNU Trondheim)

Time: Wednesday 10:45–11:45

Location: H1

KFM 8.1 Wed 10:45 H1

Hyperfine Structure of Transition Metal Defects in SiC — •BENEDIKT TISSOT and GUIDO BURKARD — Universität Konstanz

Transition metal (TM) defects in silicon carbide (SiC) are a promising platform in quantum technology, especially because some TM defects emit in the telecom band. We develop a theory for the interaction of an active electron in the D -shell of a TM defect in SiC with the TM nuclear spin and derive the effective hyperfine tensor within the Kramers doublets formed by the spin-orbit coupling. Based on our theory we discuss the possibility to exchange the nuclear and electron states with potential applications for nuclear spin manipulation and long-lived nuclear-spin based quantum memories.

KFM 8.2 Wed 11:00 H1

Exploring Binary Cesium-based Photocathode Materials via High-Throughput Density Functional Theory Calculations —

•HOLGER-DIETRICH SASSNICK¹ and CATERINA COCCHI^{1,2} — ¹Carl von Ossietzky Universität Oldenburg - Physics Department, Oldenburg, Germany — ²Humboldt-Universität zu Berlin - Physics Department and IRIS Adlershof, Berlin, Germany

Cesium-based photocathodes are commonly used as electron sources in particle accelerators; one relevant issue hindering the control over these systems and hence their photoemission performance is their polycrystalline structure which often includes non-stoichiometric compositions. To predict which compounds are more likely to form and to control their properties, we apply an efficient high-throughput workflow based on density functional theory calculations and explore the compositional phase space of cesium-based materials. First, we calculate the formation energies as well as the electronic properties of crystalline phases obtained from computational databases employing the meta-GGA functional SCAN, which is known to provide accurate results for these systems [1]. Then, we include additional crystal structures based on chemical similarity as a preliminary step towards crystal structure prediction combined with machine learning approaches. Our results indicate that a larger number of different crystal structures may be formed and thus contribute to the macroscopic material properties.

[1] Sašnick & Cocchi, *Electron. Struct.* **3** 027001 (2021)

KFM 8.3 Wed 11:15 H1

Mobility functions for [001] CSL grain boundaries in Nickel from Molecular Dynamics — •ETIENNE NGENZI, ZAKARIA EL OMARI, CHARLIE KALHOUN, BRIGITTE BACROIX, and SYLVAIN QUEYREAU — LSPM UPR 3407 CNRS, Université Sorbonne Paris Nord, 93430, Villetaneuse, France

Transition metal (TM) defects in silicon carbide (SiC) are a promising platform in quantum technology, especially because some TM defects emit in the telecom band. We develop a theory for the interaction of an active electron in the D -shell of a TM defect in SiC with the TM nuclear spin and derive the effective hyperfine tensor within the Kramers doublets formed by the spin-orbit coupling. Based on our theory we discuss the possibility to exchange the nuclear and electron states with potential applications for nuclear spin manipulation and long-lived nuclear-spin based quantum memories.

Multiscale simulations constitute a possible path to improve our understanding of the evolution of microstructures. In this work, we have systematically studied the migration of [001] CSL Grain Boundaries (GB) by Molecular Dynamics to provide input data for a mesoscale Phase Field model. We have systematically studied GB in nickel over a wide range of driving forces and temperature. To identify common features between very different GB and to sample different migration processes, we explored a large number of $\Sigma 5$, $\Sigma 13$, and $\Sigma 25$, covering symmetric pure tilt, pure twist, and mixed characters ranging from low to high misorientation angle GB. Since we systematically probed both driving force and temperature, the temperature dependence of migration was unambiguous. The response of grain boundary mobility to temperature is highly dependent on the structure of the grain boundary. Most of the studied GB show successive distinct behaviours, with an initially thermally activated regime at low driving force and temperature. When increasing the driving force, the GB velocity may transition to a linear regime. A correlation is made with the elementary migration mechanisms that are observed. A phenomenological velocity law covering the entire parameter space for each GB is proposed.

KFM 8.4 Wed 11:30 H1

Electronically driven anharmonicity in charge-density-wave materials — •ARNE SCHOBERT¹, JAN BERGES¹, ERIK VAN LOON^{1,2}, MICHAEL SENTEF³, and TIM WEHLING¹ — ¹Institut für Theoretische Physik, Bremen Center for Computational Materials Science, and MAPEX Center for Materials and Processes, Otto-Hahn-Allee 1, Universität Bremen, D-28359 Bremen, Germany — ²Department of Physics, Lund University, Lund, Sweden — ³Max Planck Institute for the Structure and Dynamics of Matter, Luruper Chaussee 149, 22761 Hamburg, Germany

Charge-density waves (CDWs) occupy an important position in the phase diagram of low-dimensional systems such as the transition metal dichalcogenide monolayers. Although a CDW can often be identified already from the undistorted structure in linear response, anharmonic effects are eventually responsible for the stabilization of the distorted phase and its precise properties. To study the mechanisms responsible for the anharmonicity, we calculate Born-Oppenheimer potential energy surfaces for lattice distortions in 1T-TaS₂, 1T-VS₂, and 2H-NbSe₂, and we establish a connection to the electronic structure of these materials.

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