MM 47: Topical session: Data driven materials design - ab initio materials design

Time: Wednesday 15:45–17:00 Location: BAR 205

Topical Talk MM 47.1 Wed 15:45 BAR 205

Finite-temperature simulations of materials properties for data-driven materials design — •Igor Abrikosov — Linköping University, Linköping, Sweden — National University of Science and Technology MISIS, Moscow 119040, Russia

A systematic knowledge-based search for new materials using data-driven approaches combined with the electronic structure theory is now established as a recognized field within condensed matter physics and materials science. We show that by means of computer experiments it is possible to obtain relevant materials parameters which are difficult, expensive or impossible to obtain in physical experiments. With these tools at hands, theory is capable to guide experimental synthesis of new materials [1] as well as discoveries of exciting phenomena with high potential for novel technologies [2]. We present new approaches that allow to bring simulations conditions much closer to those at which materials operate in tools and devices. In particular, we focus on simulations at finite temperatures and discuss the results obtained for transition metal alloys [3] as well as for transition metal nitrides [4]. We argue that using novel tools increases reliability of theory underlying data-driven materials design.

[1] A. S. Ingason, et al., Phys. Rev. Lett. 110, 195502 (2013). [2] V. Ivády, et al., Phys. Rev. Lett. 117, 220503 (2016). [3] M. P. Belov, N. V. Skripnjak, A. V. Khvan, A. Dinsdale and I. A. Abrikosov, in preparation. [4] N. Shulumba, et al., Phys. Rev. Lett. 117, 205502 (2016).

MM 47.2 Wed 16:15 BAR 205

Evolution of defect populations in silicon carbide : coupling ab initio energetics, charged defects and rate theory — •Guido Roma, Thomas Jourdan, Quentin Bouton, Jean-Paul Crocombette, and Fabien Bruneval — DEN-Service de Recherches de Métallurgie Physique, CEA, Université Paris-Saclay, 91191 Gif sur Yvette, France

Ab initio based evolution of defect populations using stochastic methods or rate theory has been developed since at least a decade and has provided the explanation of the evolution of material properties of irradiated materials [1]. Its application concerns, however, mostly metals. Although applications to semiconductors or insulators exist [2], they overlook in most cases the variety of charge states of point defects. We discuss here an approach to overcome this limitation in the case of silicon carbide, where we dispose of a relatively complete database of defect energetics. We present some results of rate theory simulations for silicon carbide where intrinsic defects are supersaturated, as it happens for example under or after electron irradiation. In particular, we show examples where the mutual influence of doping and kinetics in the material matters, and we revisit our previous prediction of SiC nanodecomposition driven by vacancy-interstitial recombinations [3], where electrostatic effects were neglected. We discuss also the possibility of coupling this approach with the simulation of spectral properties, with the example of Raman spectra.

MM 47.3 Wed 16:30 BAR 205

Optical properties of disordered graphene quantum dots — •Abdulmenaf Altintas, Korhan Çakmak, and Alev Devrim Güçlü — Department of Physics, Izmir Institute of Technology, IZTECH, TR35430, Izmir, Turkey

We investigate the effects of disorder and electron-electron interactions on the optical properties of graphene quantum dots using tight-binding, mean-field Hubbard and configuration interaction approaches. We consider hexagonal armchair quantum dots containing up to 10806 atoms, where the disorder is modelled as a long-range random potential landscape, giving rise to electron-hole puddles. We show that disorder induced electron and hole localizations near Fermi level is reduced due to electron-electron interactions, making the observation of universal optical conductance robust against imperfections. When disorder is present, calculated absorption spectrum approaches the experimental results for isolated mono layer of graphene sheet.

MM 47.4 Wed 16:45 BAR 205

First-principles insight into the martensitic transformation and diffusion properties in Ti-Ta alloys — •Tanmoy Chakraborty, Jutta Rogal, and Ralf Drautz — Interdisciplinary Centre for Advanced Materials Simulation, Ruhr-Universität Bochum, 44780 Bochum, Germany

In Ti-Ta-based high-temperature shape memory alloys (HTSMAs) the martensitic transformation temperature (M_s) exhibits a strong dependence on the chemical composition. A detailed knowledge of the underlying mechanisms and phase stability of the competing austenite and martensite phases in these alloys can aid the design of new HTSMAs with the desired functional properties at elevated temperatures. Using density functional theory in combination with the quasi-harmonic Debye model we approximate the different contributions to the free energy as a function of composition and compare the stability of competing phases at finite temperature. We identify the physical key parameters governing the experimentally observed composition dependence: the 0K energy difference and the difference in the Debye temperature between the involved phases. From our calculations we propose a one dimensional descriptor for high-throughput screening of M_s for the design of new HTSMAs. In addition to the thermodynamic phase stability we investigate the mobility of the different elements within the alloy as a function of composition and local environments which is key to analyze segregation and redistribution at elevated temperatures.