Emerging Materials for Nanophotonics and Plasmonics

Alexandra Boltasseva

School of Electrical&Computer Engineering and Birck Nanotechnology Center, Purdue University, West Lafayette, IN 47907, USA

The fields of nanophotonics and plasmonics have taught us unprecedented ways to control the flow light at the nanometer scale, unfolding new optical phenomena and redefining centuries-old optical elements. As we continue to transfer the recent advances into applications, the development of new materials has become a centerpiece in the field of nanophotonics. In this presentation I will discuss emerging material platforms including transparent conducting oxides, transition metal nitrides, oxides and carbides for future consumer-level optical components and systems across the fields of sensing, spectroscopy, communication, energy, and quantum optics.

Alexandra Boltasseva is an Associate Professor at the School of Electrical and Computer Engineering, Purdue University. Boltasseva received the 2013 IEEE Photonics Society Young Investigator Award, 2013 Materials Research Society (MRS) Outstanding Young Investigator Award, MIT Technology Review Top Young Innovator (TR35) award. She is a Fellow of the Optical Society of America (OSA), a member of MRS Board of Directors and Editor-in-Chief for OSA's Optical Materials Express.

Addressing the challenge of morphology prediction at organic/inorganic interfaces

Patrick Rinke[*]

Aalto University
School of Science, 00076 Aalto, Finland
email: patrick.rinke@aalto.fi

Identifying the arrangement of atoms and molecules at hybrid organic/inorganic interfaces has givens us insight into the properties of these interfaces and their function. In our work we use atomistic quantum mechanical simulations to map the structure of an interface onto an intrinsic energy, with lower energies indicating more stable structures. Consequently, theoretical structure or morphology prediction focuses on exploring the resulting phase-space, the complex potential energy surface (PES), with the aim to find lowest energy regions and associated structures. For hybrid interfaces this is a formidable challenge due to the vast number of possible structures and their often similar energies, which are driven by entropy and not quantum mechanics.

In this presentation, I will address this morphology challenge in two different ways. For hydrogen adsorption on the ZnO (1010) surface, we constructed a cluster-expansion from our quantum mechanical simulations that enables a fast enumeration of different structures. We find that all low free-energy configurations of atomic hydrogen on the ZnO (1010) surface are disordered at realistic temperatures and pressures. The surface phase diagram reveals a gradual transition between thermodynamically stable disordered phases of different H coverage. For C60 molecules adsorbed on the (101) surface of anatase TiO_2, I will introduce a new machine learning paradigm. This time we use our quantum mechanical calculations to train a machine to build a model of the PES using Bayesian optimization. The PES tells us the most stable adsorption sites of C60 without having to resort to chemical intuition and will let us explore the dynamic behaviour of the molecules on the surface in the future.

(*) This work was performed in collaboration with M. Todorovic, M. E. Stournara, S. Rigamonti, S. V. Levchenko, O. T. Hofmann, and M. Scheffler.