December 21, at 16:00-17:00

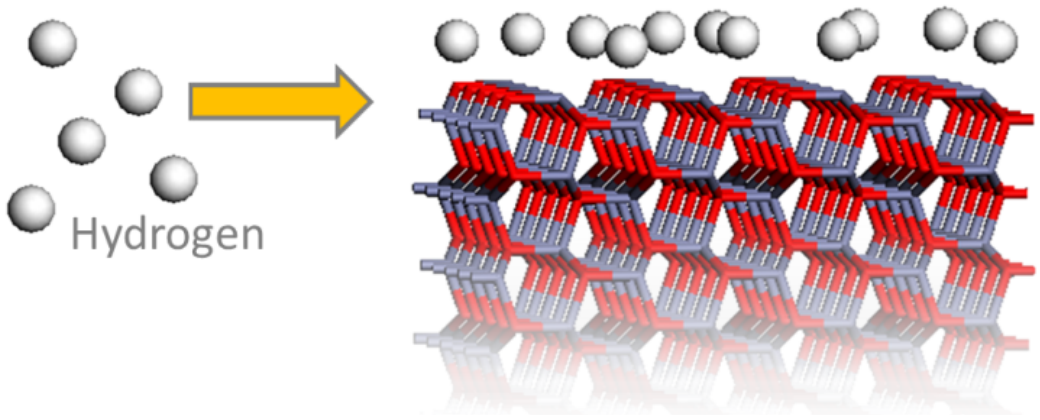
Skoltech, Blue Bldg, room 402

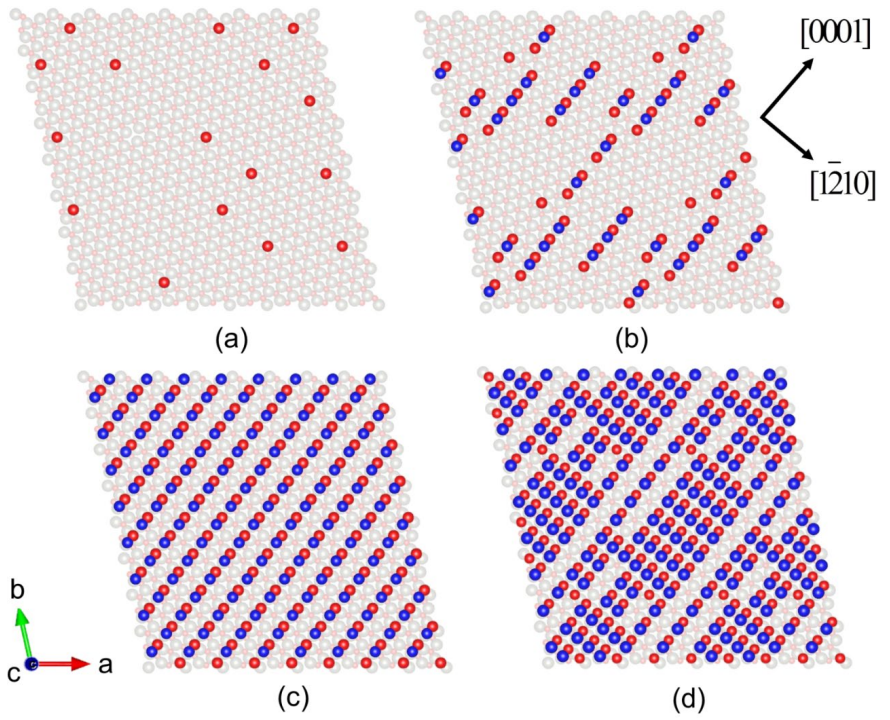
Skoltech

Skolkovo Institute of Science and Technology

Ab initio Modelling of Surfaces at Realistic Conditions:

Interplay of Adsorbate-Substrate and Adsorbate-Adsorbate Interactions





Speaker

Sergey V. Levchenko

Fritz Haber Institute of the Max Planck Society, Berlin

Abstract:

Surfaces and interfaces play increasingly important role in the design of functional materials. Such materials operate at finite temperatures and pressures, and, in order to understand and predict their behavior at realistic conditions, the effects of the external factors have to be taken into account. In this talk, I will demonstrate the importance of addressing this challenge by applying ***ab initio*** atomistic thermodynamics to explain a puzzling experimental observation of one-dimensional adsorbed water structures at CaO (001) surfaces exposed to water vapor. In another example, I will show how traces of hydrogen in the atmosphere change the structure and composition of ZnO (10-10) surface. ZnO is a promising substrate for hybrid inorganic-organic photovoltaic and electronics devices. The performance of such devices is affected by the structure and composition of ZnO surfaces. Since hydrogen is a common contaminant during and after ZnO fabrication, it is paramount to identify and predict surface phases of ZnO at realistic temperatures and partial hydrogen pressures. For both examples, I will show how a subtle interplay between adsorbate-substrate and adsorbate-adsorbate interactions plays a decisive role in the behavior of surfaces at realistic conditions.

Biography:

Sergey V. Levchenko graduated with honors in 1998 from the Moscow Institute of Physics and Technology. In 2005, he obtained Ph.D. in Chemistry from the University of Southern California. During his Ph.D., he conducted theoretical and computational studies of electronically and vibrationally excited states of molecules using quantum-chemistry methods. In 2006-2008, Dr. Levchenko has been a postdoctoral research associate in the University of Pennsylvania, where he studied surfaces of ferroelectric materials using density-functional theory and ***ab initio*** atomistic thermodynamics. Since 2008, he is a leader of the group "Unifying Concepts in Catalysis" at the Fritz Haber Institute of the Max Planck Society in Berlin, Germany. The group develops electronic-structure, statistical mechanics, and machine-learning methods for materials, and applies these methods to model surfaces and interfaces, as well as catalytic processes, at realistic temperature, pressure, and doping conditions.

LOOKING FORWARD TO SEEING YOU!