ÚSTAV INFORMATIKY
SLOVENSKÁ AKADÉMIA VIED

Pozývame Vás na

SEMINÁR ÚI SAV,

ktorý sa bude konať v utorok, 14. 2. 2017 o 9.30
v zasadačke ÚI SAV č. 102, Dúbravská cesta 9, Bratislava

Program:
Prof. Ing. Ivan Štich, DrSc,
Center for Computational Materials Science (CCMS), Institute of Physics, SAS, Institute of Informatics, SAS

Computational physics and chemistry at CCMS

Tešíme sa na stretnutie s vami pri šálke kávy alebo čaju.

Computational physics and chemistry at CCMS

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In the seminar I will focus on the recent computational projects underway in the CCMS group, especially those which have been finished during my part-time job at II SAS. The focus of the CCMS is on nanotechnology and electronic structure modeling either via the density functional theory methods (DFT) or via the ultra-accurate explicitly correlated quantum Monte Carlo methods (QMC). These methods will very briefly be introduced and their performance documented on three recent projects: 1) surface probe microscopy (SPM), 2) nanotribology, and 3) electronic and photonic properties of a 2D phosphorene.

In 1) I will show the recent experimental images of truly 3D force maps above Ge(001) surface and their simulation which shows perfect agreement with the experiments and allows for a full understanding of the experimentally measured forces, Fig. 1.

In 2) I will introduce the concept of structural superlubricity (translation without any measurable friction) and will explain the reasons why some nonaprticles do exhibit superlubricity and other don't and how modeling can aid the understanding.

In 3) I will discuss the unique tunable electronic/photonic properties of perhaps the most important novel 2D material, phosphorene. The progress is hampered partly also due to the failure to determine an accurate value of the bandgap of a free-standing single-layer phosphorene both experimentally and computationally. I will show that this missing link can be provided by use of QMC methods, which provide the ultimate, albeit unexpected, results, Fig.1.

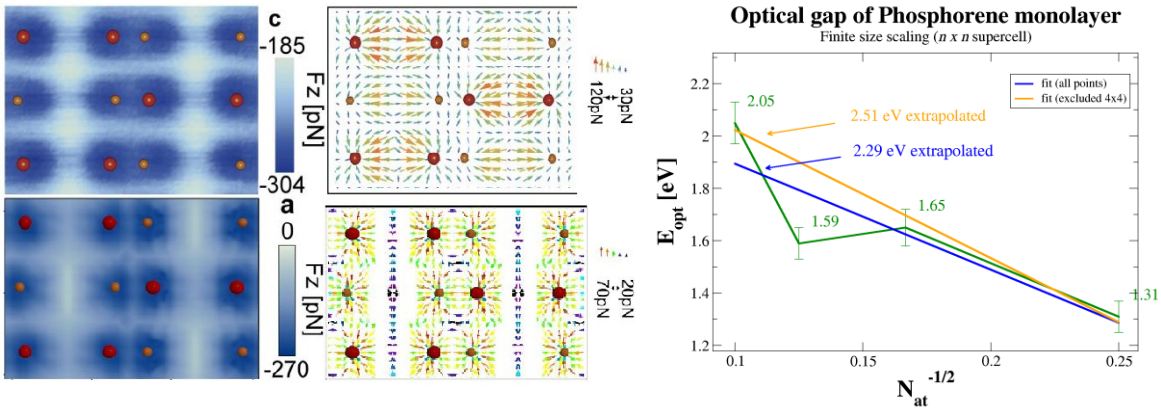

Figure 1. Left: Upper- experimental, Lower- simulated 3D force map. Right: simulated optical gap of phosphorene from QMC simulations.