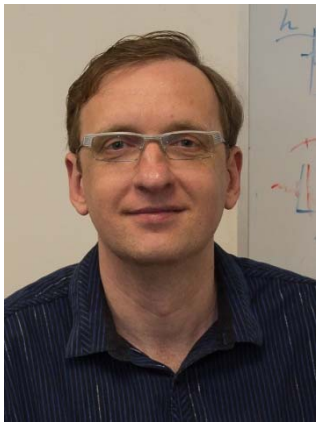
IBS Center for Multidimensional Carbon Materials

Tuesday Colloquium



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Predictive Modeling of Existing and Emerging Two-Dimensional Materials

Tuesday, MAR 14
2 PM

Bldg. 101
Seminar room on the 1st floor

Technological demand for new electronic and optical devices to replace current silicon chips has generated immense interest in two-dimensional (2D) materials, representing the ultimate size limit for conventional electronics. In addition to their great technological relevance, 2D materials also exhibit unique physical properties and new phenomena, making them an excellent testbed to study new physics in low dimensions. Beginning with graphene, 2D materials have thus emerged as an important topic of intense research. In this talk, I will focus on several of our theoretical predictions for 2D materials. First, I will discuss predicted superconductivity in 2D boron and Mo2C MXene. The former is a monoelemental single-layer material that has been recently grown on Ag surface, while the latter is a member of a large family of stable 2D transition metal carbides. We obtain electron-phonon coupling from the first principles, and, based on the microscopic BCS theory, estimate superconducting critical temperatures Tc without experimental input. We further demonstrate Tc tunability in Mo2C MXene through chemical functionalization. Together with functionalization, alloying provides a whole new degree of freedom for tunability of functional materials. As a large number of 2D alloys are currently probed combinatorially in experiment, a more guided theoretical support is called for, to allow new materials discovery in shorter time and at a lower cost. Next, we utilize the cluster expansion method to efficiently handle the combinatorial diversity of various 2D alloys: transition metal dichalcogenides, graphene, boron nitride, silicene, etc. We obtain band gaps and other electronic structure parameters as well as thermodynamic stabilities that agree favorably with available measurements. I will finally address new scaling and carrier delocalization behaviors in lateral in-plane 2D p-n junctions governed by their low dimensionality.

You are cordially invited to attend!