IBS Center for Multidimensional Carbon Materials

Special Guest Seminar

Prof. Boris I. Yakobson

Karl F. Hasselmann Chair in Engineering
Materials Science and NanoEngineering,
Chemistry and Richard E. Smalley Institute
Rice University, Houston, USA

Predictive modeling of low-dimensional materials, synthesis to properties

MAY 24
THUR 2 PM

Bldg. 101
Seminar Room on the 1st floor

Comprehensive tools of materials modeling allows one to make verifiable predictions of novel physical structures with specific, often useful or even extraordinary, properties. Recent examples from our work at my Rice University (Fig. 1) lab will be presented. First, an outlie of evolutionary selection growth of monocrystal achieved for graphene [1] and how it should work particularly efficiently for other binary compositions of lower symmetry, like h-BN or metal dichalcogenides. I will only briefly discuss 2D boron, a.k.a. borophene, which is now well covered by our reviews [2]. But will focus instead on MX2 family, where a combination of DFT and phase-field simulations proves useful for understanding planar [3] and even non-Euclidean growth on nonplanar substrates [4], with intentional defect design for bringing new functionality. I will also share a few-years long saga on how we went from defining an efficient electronic structure descriptor "E_{lus}" to identifying best TMD-candidates and to experimental verification of their catalytic efficiency for HER [5].

References:

1. Vlassiouk et al. *Nature Mater.*, 17, 318 (2018) || Passerone, "Grown with the wind", *Nature Mater.*, 17 , 296 (2018).
2. Zhang, Penev, BIY, *Nature Chem.*, 8, 525 (2016) || idem. *Chem. Soc. Rev.* 46, 6746 (2017) || A. Mannix et al. *Nature Nanotech.*, in press (2018).
3. Artyukhov, Hu, et al. *Nano Lett.* 16, 3696 (2016) || J. Zhou et al. *Nature*, 556, 355 (2018).
4. Yu et al. *ACS Nano*, 11, 8612–8618 (2017).
5. |Liu et al. *Nature Energy*, 2, 17127 (2017).

You are cordially invited to attend!