Seminar

Predictive modeling of low-dimensional materials, synthesis to properties

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Venue: w563, Physics building, Peking University

地点：北京大学物理楼，西563会议室

Abstract

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 outline 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].

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).

About the Speaker

Boris I. Yakobson is an expert in theory and computational modeling of materials nanostructures, of their synthesis, mechanics, defects and relaxation, transport and electronics. Presently, Karl F. Hasselmann Endowed Chair in Engineering, professor of Materials Science and Nano-Engineering, and professor of Chemistry, Rice University, Houston, Texas. Received PhD 1982 in Physics and Applied Mathematics, from Russian Academy of Sciences. 1982-1989, Head of Theoretical Chemistry lab at the Institute of Solid Materials of the Russian Academy. 1990-1999, on the faculty of the Department of Physics, North Carolina State University. His research, sponsored over the years by the National Science Foundation, Department of Energy, NASA, Department of Defense, Army Research Office, Air Force Research Laboratory and AFOSR, Office of Naval Research, as well as private industry and foundations, resulted in over 400 publications and eight patents. Received Department of Energy Hydrogen Program Award, Nano 50 Innovator Award from Nanotech Briefs (Boston), Royal Society (London) Professorship Award, Department of Energy R & D Award, NASA Faculty Award. Yakobson has mentored a number of PhD students and postdoctoral associates, serves on the editorial boards of several journals and on steering committees.

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