allied academies

International Conference on

Nanomaterials and Nanotechnology

October 29-30, 2018 | London, UK

Predictive modelling of low-dimensional materials: Synthesis to properties

Boris I Yakobson
Rice University, USA

Comprehensive tools of materials modelling allow one to make verifiable predictions of novel physical structures with specific, often useful or even extraordinary, properties. Recent examples from our work will be presented. First, briefly about evolutionary selection growth of monocrystal achieved for graphene and how it should work particularly efficiently for other binary compositions of lower symmetry, like h-BN or metal dichalcogenides. I will skip all 2D boron, borophene, because it is given to different Symposium. But will focus instead on MX_2 family, where a combination of DFT and phase-field simulations proves useful for understanding planar and even non-Euclidean growth on nonplanar substrates, 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 "Elus" to identifying best TMD-candidates and to experimental verification of their catalytic efficiency.

e: biy@rice.edu

Notes: