MAR17-2016-020451

Abstract for an Invited Paper
for the MAR17 Meeting of
the American Physical Society

Predictive modeling of 2D materials, from synthesis to properties[1]

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Comprehensive tools of materials modeling are derived from the principles of physics and chemistry, empowered by high performance computing. Together, this allows one to make verifiable predictions of novel physical structures with specific, often useful or even extraordinary, properties. Examples from our work will be presented, first being growth and unusual morphology of binary compositions of metal dichalcogenides MX2 [1], where a combination of DFT and phase-field simulations proves useful. Second, prediction of pure mono-elemental boron 2D B and its particular structures, which culminated in recent experimental confirmations, while also promises new 2D-superconductor [2]. We will also discuss its physical properties like superconductivity [2] or plasmonics [2]. Third, we will discuss new physics emerging in heterojunctions, in either stacked or coplanar configurations [3]. [1] V. Artyukhov et al. Phys. Rev. Lett. 114, 115502 (2015) ||V. A. - Z.Hu et al. Nano Lett. 16, 3696 (2016). [2] Z. Zhang et al. Nature Chem. 8, 525 (2016) ||Z. Zhang et al. Angewandte Chemie Int. Ed. 54, 13022 (2015) ||E. Penev - A. Kutana et al. Nano Lett. 16, 2522 (2016) ||Z. Zhang, Nano Lett. 6, 6622 (2016) ||A. Brotchie, Nature Reviews, doi:10.1038/natrevmats.2016.83 (2016) ||S. Shirodkar, Y. Huang et al. (unpublished). [3] J. Yuan, Z. Zhang et al. ACS Nano, 9, 555 (2015) ||H. Yu, A. Kutana et al. Nano Lett. 16, 5032 (2016).

[1]The work was supported by the Department of Energy, the Office of Naval Research, and the Army Research Office.