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Predictive modeling of 2D materials, synthesis to properties

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Abstract: The 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. Recent examples from our work will be presented. First, briefly about growth and unusual morphology of graphene [1] or binary compositions of *metal dichalcogenides* MX_2 [2], 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 [3]. We may also mention, if time permits, its physical properties like superconductivity [3], detected Dirac cone dispersion, plasmonics, and catalysis [3].

[1] V. Artyukhov et al. **Phys. Rev. Lett.** 114, 115502 (2015).

[2] V. A. - Z.Hu et al. **Nano Lett.** 16, 3696 (2016).

[3] 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 et al. **Nano Lett.** 6, 6622 (2016) || A. Brotchie, **Nature Reviews**, doi:10.1038/natrevmats.2016.83 (2016) || S. Shirodkar, Y. Huang et al. (unpublished) || Y. Liu et al. **Nature Energy** 2, 17127 (2017).

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