Computational modeling and discovery of two-dimensional materials and vdW heterostructures

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The family of atomically thin two-dimensional (2D) materials, which started with graphene, has expanded rapidly over the past few years and now includes insulators, semiconductors, metals, ferromagnets, and superconductors. This development has prompted an explosion in envisioned applications ranging from batteries and catalysis to photovoltaics, electronics, and photonics. In parallel with this development, the possibility of stacking different 2D materials into van der Waals heterostructures has opened new routes for designing atomically flat heterostructures with tailored properties. I will show how the electronic and optical properties of 2D materials and their heterostructures can be accurately predicted by combining many-body quantum mechanics and high-performance super computing. I will give examples from our recent research focusing on tunable excitons[1-2], long-lived plasmons [3] and light with hyperbolic dispersion relations[4] – all realized by means of vdW bonded 2D materials. Finally, I will present our recent efforts to establish a comprehensive computational database of more than one thousand 2D materials using an efficient and semi-automatic high-throughput framework [5] (http://c2db.fysik.dtu.dk).

References:

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