First principle calculations of excitonic phases in van der Waal heterostructures

Fredrik Nilsson
Kristian Thygesen
CAMD, Technical University of Denmark (DTU), DK-2800 Kgs. Lyngby, Denmark
fanni@dtu.dk

Computational materials discovery has played a major role in the discovery of novel two dimensional materials, such as e.g. transition metal dichalcogenides. Different monolayers can be combined to form heterostructures with even richer phase diagrams. One interesting phenomenon in these heterostructures are long lived excitons formed by spatially separated electron-hole pairs. In double bilayer graphene experimental evidence of exciton condensation we found 2018 [1] while MoSe2/WSe2 bilayers have been shown to become excitonic insulators at certain electron and hole concentrations [2]. In both of these experimental setups the electron hole layers were separated by hBN barriers and the electron and hole concentrations were tuned using external gates. In this talk we will discuss how the newly developed excitonic density functional theory method [3] can be combined with the quantum electrostatic heterostructure model [4] to allow for realistic computations of the excitonic properties of stacked 2D materials. We will show how the relative band alignment as well as intrinsic dipole moments of some of these materials can be used to tailor their properties, without the need for hBN barriers or external fields, and propose new material combinations with interesting excitonic phases.

References

[1] W. Burg et. al Phys. Rev. Lett. 120 (2018)
[2] L. Ma et al, Nature 598 (2021)
[3] F. Nilsson et. al. Phys. Rev. Mat. 5 (2021)
[4] K. Andersen et al Nano Lett. 15 (2015)

Figures

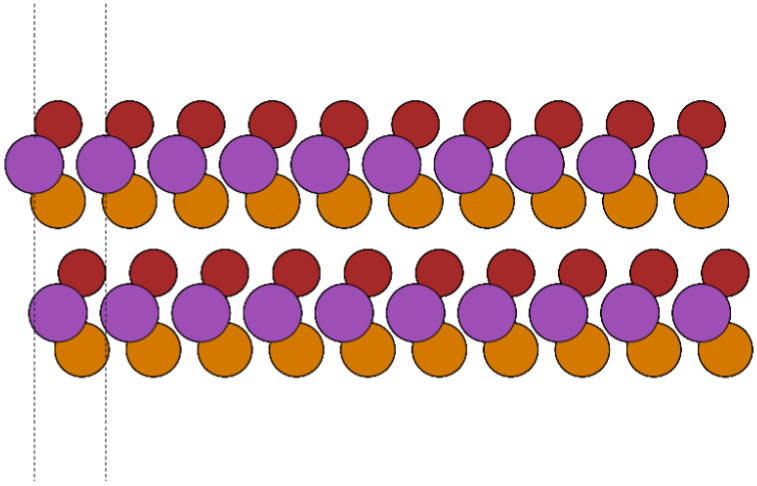

Figure 1: Schematic figure of a Janus bilayer