Interlayer interactions and the electronic and optical properties of 2D multilayer materials

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Despite largely non-covalent interlayer interactions, the electronic and optical properties of stacked homo- and hetero-multilayers of 2D materials can show an interesting variation with the twist angle due to differences in the crystal potential and symmetry breaking. In principle, this offers the possibility to tailor the physical properties of interest of composite materials through variation of the relative alignment of the constituting materials. In this talk, I will explore the effect of stacking order for two bilayer materials: For $MoSe_2/WSe_2$ heterobilayers, the local stacking order leads to small variations in the hybridization between the $MoSe_2$ and WSe_2 bands and has a decisive effect on the polarization dependence of the momentum-direct interlayer excitonic absorption, while the interlayer exciton binding energies are only weakly affected [1]. For stacked homo-bilayers of antimonene, I will show that the interlayer interaction has a significant covalent contribution [2]. The residual bonding effects result in a closing of the indirect electronic band gap for AB stacking and small twist angles, which can be lifted for larger twist angles.

[1] Gillen et al., Phys. Rev. B 97, 165306 (2018)

[2] Gibaja et al., Angewandte Chemie Int. Ed. 55, 14345 (2016)