**Electronic and Optical Properties of 2D-material-based Heterostructures**

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The atomically thin nature of layered two-dimensional (2D) materials results in emerging properties that are different from their bulk counterparts. One often cited example is the reduced electronic screening resulting in stronger exciton binding energies in 2D materials. 2D materials are also interesting because of the potential for bottom-up design of various flexible heterostructures. In this regard, it is important to understand how the different components of the heterostructure affect the electronic and optical properties of the system. We will discuss 2D-material heterostructures based on the elemental material phosphorene, as well as hybrid organic-2D-material heterostructures. Using state-of-the-art GW+BSE methods, we show that bright interlayer excitons exist in the direct band gap phosphorene (BP)-based heterostructures (BP/GeS and BP/hBN), with a good compromise between binding energies, oscillator strength and radiative lifetimes.[1] Strong hybridization between GeS and BP increases the effective mass and room temperature exciton lifetimes, while the hBN spacer layer decouples the BP monolayers in BP/hBN/BP, resulting in the lowest energy exciton becoming dark. A single hBN layer reduces the exciton binding energy in monolayer BP by ~0.11 eV, while adding another hBN layer in hBN/BP/hBN further reduces the binding energy by ~0.03 eV. This brings us to our next topic, which is to investigate how a 2D material screens excitations *adjacent to* it, such as excitations in adsorbed molecules. We show that the extent to which a material screens the band gap of small adsorbed benzene molecules is given by the screening potential Vscr(r,r) at the position of the molecule. Interestingly, by computing Vscr(r,r) for a range of 2D materials and slabs of 3D materials, we find that Vscr(r,r) at a given distance away from the material scales approximately linearly with the quasiparticle gap in the same manner for all these materials. This is in contrast to the screening of excitations within materials, which differ significantly between 2D and 3D materials. Finally, if time permits, we will discuss Raman optical spectra for organics on 2D materials, where electron-phonon coupling leads to interesting chemical enhancement effects.

1. Y. Chen, and S. Y. Quek, 2D Materials **5**, 045031 (2018).