Modelling Excitons in Atomically Thin Semiconductors

Simone Latini, Thomas Olsen, Kristian S. Thygesen

Center for Atomic-Scale Materials Design, Department of Physics Technical University of Denmark
Fysikvej 311, 2800 Kgs. Lyngby
simola@fysik.dtu.dk

Despite the numerous extraordinary properties of pristine graphene, its application to (opto)-electronics is problematic due to the lack of a band gap. This issue inevitably requires the systematic research for new materials which combine a strong 2D nature and a semiconducting behaviour. As soon as a band gap is opened, excitonic effects start to play a fundamental role on the optical properties determining, for example, the onset of the optical transitions. The Bethe-Salpeter Equation (BSE) is nowadays the most refined method to quantitatively describe excitons but its applicability is limited to relatively simple systems because of its computational complexity. Here we propose a simple method to estimate the energy of the lowest bound exciton based on a modified Mott-Wannier model. For 2D semiconductors the dielectric function turns out to be strongly dependent on the wave vector and therefore the definition of the value for the dielectric constant to plug into the hydrogenic model has to be revised. This is done accounting for a quasi-2D picture of the exciton. The validity of the method is checked thoroughly benchmarking the binding energies and exciton radii for a large variety of 2D materials against the values obtained from the solution of the BSE. Our method has the merit to both keep the computational cost low and to provide a straightforward physical intuition on excitonic effects.