Nature of Excitons in Bidimensional WSe_2 by Hybrid Density Functional Theory Calculations

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Abstract

2D tungsten diselenide (2D-WSe_2) is one of the most successful bidimensional materials for optoelectronic and photonic applications, thanks to its strong photoluminescence properties and to a characteristic large exciton binding energy. Although these optical properties are widely recognized by the scientific community, there is no general understanding of the atomistic details of the excitonic species giving rise to them. In this work, we present a density functional theory investigation of excitons in 2D-WSe_2, where we compare results obtained by standard generalized gradient approximation (GGA) methods (including spin-orbit coupling) with those by hybrid density functionals. Our study provides information on the size of the self-trapped exciton, the number and type of atoms involved, the structural reorganization, the self-trapping energy, and the photoluminescence energy, whose computed value is in good agreement with experimental measurements in the literature. Moreover, based on the comparative analysis of the self-trapping energy for the exciton with that for isolated charge carriers (unbound electrons and holes), we also suggest a simplified approach for the theoretical estimation of the excitonic binding energy, which can be compared with previous estimates from different approaches or from experimental data.

References

[1] H. Liu, P. Lazzaroni, C. Di Valentin, Nanomaterials, 8 (2018) 481.

Figures

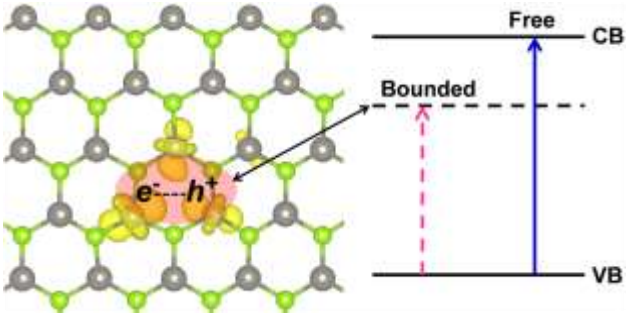

Figure 1: Schematic representation of the exciton in WSe_2.