Stacking-Dependent Interlayer Excitons in BP/$CrSe_2$ van der Waals Heterostructure

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The emergence of two-dimensional van der Waals (vdW) heterostructures has revolutionized exciton-based research due to their tunable electronic and optical properties. Here, we present a systematic many-body study of a BP/$CrSe_2$ vdW heterostructure composed of experimentally realized boron phosphide (BP) and chromium diselenide ($CrSe_2$) monolayers. We find a robust type-II band alignment across all stacking configurations; however, interlayer excitons emerge selectively depending on the stacking order [1]. The vdW heterostructure exhibits strong exciton binding energy (0.34–0.44 eV, depending on stacking) and nanosecond-scale room-temperature radiative lifetimes, indicating long-lived excitonic states. Additionally, its optical absorption extends from the visible to the near-infrared regime, underscoring its potential for optoelectronic and excitonic applications. Our findings highlight the critical role of stacking-dependent interlayer coupling in controlling the excitonic properties of vdW heterostructures, paving the way for tailored design strategies in next-generation light-harvesting and quantum technologies.
From a computational point of view, our work uses very accurate many-body methods (GW, BSE, TD-DFT) to resolve delicate effects, such as the interplay between electron-electron and electron-hole interaction, which we proved to be precise at the experimental level [2-3] or compatible with independent stochastic approaches (QMC) [4-5] also for 2D materials.

References

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Figures