

Tunable dipolar and exchange interactions of Charge Transfer Excitons in Lateral TMD heterostructures

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Abstract

Charge Transfer (CT) excitons comprising of spatially separated electrons and holes, have recently been theoretically predicted and experimentally observed in lateral heterostructures of transition metal dichalcogenides (TMDs) (Rosati, R. et al. Nat. Commun. 14, 2438 (2023)). These CT excitons exhibit unique transport phenomena across and along the interface of the lateral heterostructures. However, the microscopic many-particle processes behind transport and dynamics of CT excitons have not been completely understood. Here, we study exciton-exciton interactions of bound CT excitons in hBN-encapsulated WSe_2 - MoSe_2 lateral heterostructures. We show that variation of energy band offset considerably changes the localization of center of mass and dipole, leading to a transition of the CT excitons to monolayer excitons. The band offset plays the key role, and we find a critical value of 100 meV of the energy band offset, below which CT excitons become negligible, and we obtain the behavior of monolayer excitons. Our results demonstrate a blueshift due to repulsive dipolar interactions, and a redshift due to attractive exchange interaction for bound CT excitons with a net density-dependent blueshift in the range of tens of meV. For low band offsets, the behavior of exciton-exciton interactions and the resulting energy renormalization corresponds to that of monolayer excitons as reported in Erkensten, D. et al., Phys. Rev. Materials 6, 094006 (2022).