Interlayer Trions in the MoS2/WS2 van der Waals Heterostructure

Electronic excitations in van der Waals heterostructures can have interlayer or intralayer character depending on the spatial localization of the involved charges (electrons and holes). In the case of neutral electron-hole pairs (excitons), both types of excitations have been explored theoretically and experimentally. In contrast, studies of charged trions have so far been limited to the intralayer type. Here we investigate the complete set of interlayer excitations in a MoS2/WS2 heterostructure using a novel ab initio method, which allows for a consistent treatment of both excitons and trions at the same theoretical footing. Our calculations predict the existence of bound interlayer trions below the neutral interlayer excitons. We obtain binding energies of 18/28 meV for the positive/negative interlayer trions with both electrons/holes located on the same layer. In contrast, a negligible binding energy is found for trions which have the two equally charged particles on different layers. Our results advance the understanding of electronic excitations in doped van der Waals heterostructures and their effect on the optical properties.