THEORETICAL INVESTIGATIONS OF OPTICAL PROPERTIES OF 2D SEMICONDUCTORS IN VAN DER WAALS HETEROSTRUCTURES

I. Gerber[1]

[1]Université de Toulouse, INSA–CNRS–UPS, LPCNO, Toulouse F-31077, France

Stacking 2D materials to build van der Waals heterostructures provides an interesting approach toward creating artificial lattices with desired band structures and possible new functionalities. In transition metal dichalcogenide (TMD) monolayers the optical absorption is strong, but the transition energy cannot be tuned as the neutral exciton has essentially no out-of-plane static electric dipole. In contrast, for homo-bilayers systems hole delocalization over the bilayer is only allowed in *2H* stacking and results in strong interlayer exciton absorption and also in a larger A-B exciton separation as compared to *3R* bilayers [1]. *GW*+BSE calculation scheme confirm signatures of efficient interlayer coupling for *2H* stacking for the MoS_2 bilayer case [2], when theoretical investigations of interlayer exciton properties for others TMD bilayers show interesting features. Besides, interlayer exciton transitions are widely tunable in applied electric fields [3] allowing to investigate the interaction between intra and interlayer excitons [4].

References

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corresponding author : igerber@insa-toulouse.fr