Optical Spectra and Excitonic Effects in Hetero-Stacked Layers of Transition Metal Dichalcogenides

Transition metal dichalcogenides (TMD) form bulk materials with single layer constituents interacting through van der Waals forces that show metallic, semiconductive to insulating behavior. In particular, the insulating family of TMD is characterized by indirect electronic gaps in the bulk crystals that are found to switch to direct gaps when free-standing single layers (SL) are considered[1].

The very recent advances in experimental procedures to synthesize SL atomic crystals[2] have paved the way for a new effort in exploiting the different properties that 2-dimensional TMD can exhibit in terms of optical absorption, tensile strain, electron doping, and multi-stacking. Thanks to the small building block (chemical formula MX_2, M metal and X chalcogenide) and thus reduced size of the theoretical models to implement for analyzing and predict the properties of these SL TMD, a growing literature is emerging where the electronic and optical properties have been addressed[3]. A lot of work is still needed, given the ongoing availability of new results where the possibility to stack several SL to form sandwiches or multi-layered TMD can lead to continuous tuning of optical properties[4]. Optoelectronic applications are thus the natural final target for this class of (quasi-)2D materials, where fundamental elements are the thermodynamic stability, the absorption and transport efficiencies.

In this talk we will address the effects of the inclusion of dynamic and static screening on the electronic states for the band dispersion properties and on the electron-hole couples for the optical absorption spectra. In particular, we will address the spatial localization and charge transfer properties of the excitons for multilayered TMD (M=Mo, W; X= S, Se), where the bandgap is still direct.

[1] C. Ataca, H. Sahin and S. Ciraci, J. Phys. Chem. C, 2012, 116, 8983.
[2] K. S. Novoselov, et al., Proc. Natl. Acad. Sci. U.S.A., 2005, 102, 10451.
[3] P. Johari and V. B. Shenoy, ACS Nano, 2011, 7, 5903; A. Ramasubramaniam, Phys. Rev. B, 2012, 86, 115409.
[4] K. He, et al., arXiv:1305.3673, to appear in Nano Letters; H. Terrones, F. Lopez-Urias and M. Terrones, Scientific Reports, 2013, 3, 1549.