# Understanding bound electronic excitations in graphene-related materials

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Among low-dimensional materials graphene-related structures like carbon nanotubes, hexagonal boron nitride, or transition metal dichalcogenide monolayers like $MoS_2$ are promising candidates for next-generation opto-electronic with optical properties which are dominated by excitons. In the presence of additional charges due to doping by a substrate or vacancies, trions (i.e. charged excitons) can occur in the optical spectrum. This opens a route towards a specific manipulation of the properties by light and by charging, e.g., due to an externally applied gate voltage.
Recently, we have developed a first-principle many-body approach [1] based on the framework of many-body perturbation theory for excited electronic states [2,3] which is able to describe excitons and trions on equal footing. Here, we apply this method to different graphene-related materials and discuss their spectra, energy compositions, and correlated wave functions (see Figs. 1, 2). E.g., for CNTs, or $MoS_2$ we find optically active trions red-shifted compared to the excitons, confirming experimental findings [4]. In addition, we look for further materials with strong influence of trions.

References

[1] T. Deilmann, M. Drüppel, and M. Rohlfing, Phys. Rev. Lett. **116** (2016), 196084.
[2] G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. **74** (2002), 601-659.
[3] M. Rohlfing and S. G. Louie, Phys. Rev. B **62** (2000), 4927-4944.
[4] Mak et al., Nature Materials **12** (2013), 207-213.

Figures

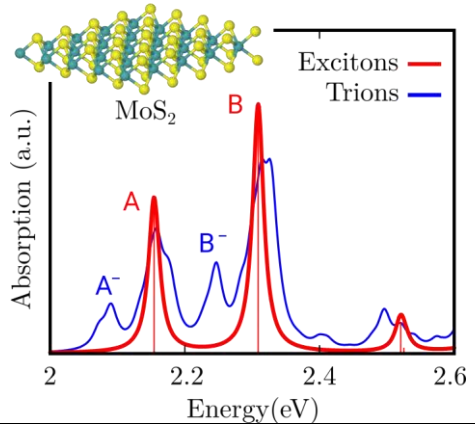


**Figure 1:** Optical luminescence in $MoS_2$ by excitons (red) and trions (blue).

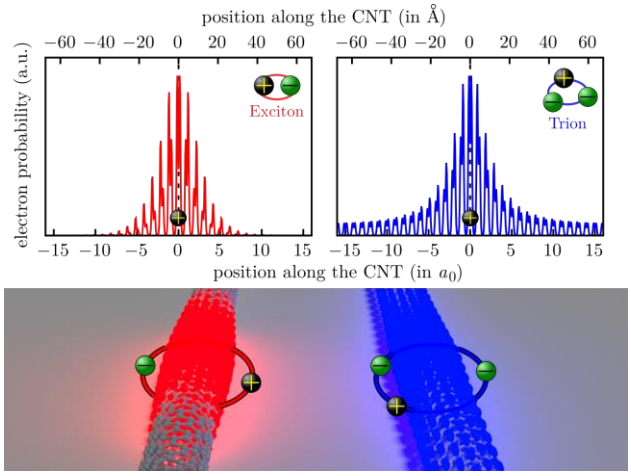


**Figure 2:** Electron probability along an (8,0) CNT for the lowest bright exciton (red) and trion (blue) along the tube and in three dimensions.