Exciton, trions and other exciting properties of single-layer MoS_2 – with and without support

Talat S. Rahman*
Department of Physics, University of Central Florida, Orlando, FL 32816

Single layer Molybdenum disulfide (MoS_2) appears to be a promising material for next generation applications owing to its low-dimensionality and intrinsic direct band-gap of about 1.9 eV. Several experimental groups have reported novel electronic and transport properties. Efforts are underway to also grow the material on support (copper, silica, boron nitride, etc.). We have carried out density functional theory (DFT) based calculations, to provide a fundamental understanding of some of the characteristics of this material. In this talk I will present our results for the binding energies of exciton and trion of a single layer of MoS_2 obtained from our version of time-dependent DFT formalism. Several types of exchange-correlation (XC) kernels are implemented in our code to compare their performance. As expected our results depend crucially on the XC kernels used. We have generalized the approach to consider the case of trion excitations, and find its binding energy to be ~0.3eV with LDA. On the other hand, we demonstrate that the results for the experimental binding energies can be reproduced by using phenomenological local and long-range XC kernels. To examine the effect of defect, I will present results for a single-layer MoS_2 with a sulfur vacancy row which shows the emergence of a defect state in the band-gap. This state is unoccupied and localized at the vacancy row. In the same vain, we find that mirror joined-edge defects formed between two MoS_2 domains exhibit metallic behavior. More interestingly, we find signatures of magnetism at specific joined-edge defects formed between two sulfur edges with 0% sulfur coverage. From the analysis of the geometric structure, I will show that some joined-edge defects undergo (2 x 1) reconstructions. I will present the implications of the above findings on electronic, transport and catalytic properties of the material and their relevance to ongoing experiments in several labs. I will also summarize our findings on the role of the support (several metal surface and BN(0001)) on the characteristics of MoS_2.

*Work done in collaboration with D. Le, V. Turkowski, T. Rawal and A. Ramirez (UCF), L. Bartels (UC Riverside) and T. Heinz (Columbia), and support in part by DOE.