TAILORING CHEMICAL AND OPTICAL PROPERTIES OF 2D TRANSITION METAL DICHALCOGENIDES

Talat S. Rahman

Department of Physics, University of Central Florida, Orlando, FL 32816, USA

Single-layer of molybdenum disulfide (MoS_2) and other transition metal dichalcogenides (TMDC) appear to be promising materials for next generation applications (optoelectronic and catalysis), because of their low-dimensionality and intrinsic direct band-gap which typically lies in the visible spectrum. Several experimental groups have already reported novel electronic and transport properties which place these materials beyond graphene for device applications. MoS_2 is also known to be a leading hydrodesulfurization catalyst. Efforts are underway to further tune these optoelectronic and catalytic properties through alloying, defects, doping, coupling to a substrate, and formation of bilayer stacks (homo- and hetero-structures). In this talk I will present results from joint theoretical and experimental investigations [1-3] which provide a framework for manipulating the functionality of this wundermaterial and take us closer to the goal of rational material design. With emphasis on the chemical properties of defect-laden single layer MoS_2, I will examine modulations in its local atomic environment (see Fig. 1 for an example) under which it could serve as a catalyst for the conversion of synthetic gas (CO and hydrogen) to methanol. With regard to the optical properties, I will present results of our analysis of the excitation spectrum and the ultrafast charge dynamics in both single- and bi-layer TMDCs obtained through the application of combined time-dependent density functional theory and many-body theory approach. In particular, I will show how the reduced electron screening in these systems leads to surprising large binding energy of electronic bound states [4] - excitons (hundreds of meVs), trions (tens of meVs) and biexcitons, in rather good agreement with available experimental data. I will also show that ultrafast (10-100fs) transfer processes are possible in these materials as a result of strongly-delocalized hole orbitals. Possible technological applications will be discussed.

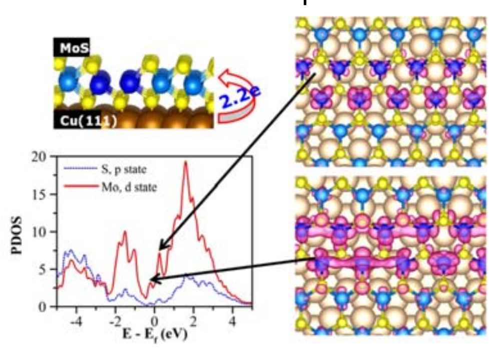

Fig. 1. Single layer MoS_2 grown on Cu(111)

Single-layer molydenum disulfide*:* transition metal dichalcogenide; exciton; catalysis

References

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