Tailoring Properties of Single Layer Transition Metal Dichalcogenides: Looking Beyond Graphene*

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Single-layer of molybdenum disulfide (MoS_2) and other transition metal dichalcogenides appear to be promising materials for next generation nanoscale 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 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 hetro-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. My emphasis will be on the structural, optical and catalytic properties of pure and defect-laden single layer MoS_2 and their possible technological applications.

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[1] D. Sun, et al., "An MoSx Structure with High Affinity for Adsorbate Interaction," Angew. Chem. Int. Ed. 51, 10284 (2012).
[2] D. Le, T. B. Rawal, and T. S. Rahman, "Single-Layer MoS2 with Sulfur-Vacancies: Structure and Catalytic Application," J. Phys. Chem. C 118, 5346 (2014).
[3] T. Komesu, D. Le, et al., "Occupied and unoccupied electronic structure of Na doped MoS_2(0001)," App. Phys. Lett. 105, 241602 (2014).