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**Tailoring properties of single layer transition metal dichalcogenides: looking beyond graphene**[1]

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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 material 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. [1] D. Sun, et al., Angew. Chem. Int. Ed. 51, 10284 (2012). [2] D. Le, T. B. Rawal, and T. S. Rahman, J. Phys. Chem. C 118, 5346 (2014). [3] T. Komesu, D. Le, et al., App. Phys. Lett. 105, 241602 (2014).

[1]Work done in collaboration with D. Le, V. Turkowski, T. Rawal and A. Ramirez and supported in part by DOE grants DE-FG02-07ER15842 DE-FG02-07ER46354