# Tuning properties of 2D materials: old dog with tricks

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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. $MoS_2$ is also known to be a leading hydrodesulphurization catalyst, for reasons that remain elusive. 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 some results which provide a framework for manipulating the functionality of these interesting van der Waals materials. With regard to 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. In particular, I will show how the reduced electron screening in these systems leads to surprisingly large binding energy of excitons (hundreds of meVs), trions (tens of meVs) and biexcitons (tens of meVs), in rather good agreement with available experimental data. I will also show that ultrafast (10-100 fs) transfer processes are possible in these materials as a result of strongly-delocalized hole orbitals. With emphasis on the chemical properties of defect-laden single layer $MoS_2$ and *h*-BN, I will examine modulations the local atomic environment under which these inert materials could serve as a catalyst for several technologically important reactions