Fast relaxation of photo-excited carriers in 2D transition metal dichalcogenides

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Monolayer transition metal dichalcogenides (TMDCs) possess unique properties [1], making them promising for creating nm-thin optoelectronic devices [2]. Understanding the process of energy relaxation in these materials is of particular importance for optoelectronics applications. We analyse the phonon mediated cooling of hot carriers in TMDCs focusing on two modes coupled to the intra-band, intra-valley relaxation process: the in-plane longitudinal optical (LO), and the out of plane

homopolar (HP) phonon modes. We predict a fast relaxation of photo-excited carriers in TMDCs, which is mediated primarily by the emission of LO phonons. By evaluating the Born effective charges for MoS₂, MoSe₂, WS₂, and WSe₂, and the corresponding LO phonon couplings, we find that, due to the polar coupling of electrons with LO phonons, the cooling times for hot electrons and holes from excitation energies of several hundred meV are at ps-scale.

[1] Qing Hua Wang, Kourosh Kalantar-Zadeh, Andras Kis, Jonathan N. Coleman, Michael S. Strano, Nature Nanotechnology, **11**, (2012), 699.

[2] Deep Jariwala, Vinod K. Sangwan, Lincoln J. Lauhon, Tobin J. Marks, Mark C. Hersam, ACS Nano, **2**, (2014), 1102.