Charge density waves and superconductivity in bulk and monolayer transition-metal dichalcogenides

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With layered structures similar to graphite, transition-metal dichalcogenides (TMD) have versatile electronic properties and rich phase diagrams that can include charge density wave (CDW) formation, superconductivity, and Mott transitions. Exfoliation of these materials to thin flakes or monolayers can yield nontrivial changes in the electronic and vibrational spectra due to quantum confinement and the reduction of interlayer interactions. In this talk, density functional theory studies of the CDW instabilities in TMDs like TaS_2, $TaSe_2$, $NbSe_2$ will be discussed. The CDW instability, which arises from an interplay between the momentum dependence of the electron-phonon interaction and that of the electronic response function, can differ in the monolayer compared to the bulk. I will also discuss the possibility of phonon-mediated superconductivity in doped single-layer MoS_2, where we find that the electron-phonon interaction can be significantly enhanced by bringing the appropriate combination of electronic states to the Fermi level.