Ab initio simulations for electronic properties and structural instabilities in condensed matter

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Transition metal dichalcogenides (TMDs) display a rich variety of instabilities such as spin and charge orders, Ising superconductivity, and topological properties. Their physical properties can be controlled by doping in electric double-layer field-effect transistors (FET). However, for the case of single layer $NbSe_2$, FET doping is limited to $\approx 1 \times 10^{14}$ cm^{-2}.[1,2] In this talk I will show, by presenting angle-resolved photoemission spectroscopy, scanning tunneling microscopy, quasiparticle interference measurements, and first-principles calculations, that a misfit compound formed by sandwiching $NbSe_2$ and LaSe layers behaves as a $NbSe_2$ single layer with a rigid doping of 0.55–0.6 electrons per Nb atom or $\approx 6 \times 10^{14}$ cm^{-2}.[3]

In the second part of my talk, I will present recent results on CuTe. This compound, called vulcanite, is one of the prototypical quasi1D systems that can be viewed as a quasi-1D CDW system with Peierls-like distortion which undergoes a CDW transition at T_{CDW} = 335 K.[4,5] In order to provide additional theoretical insights into the CDW phase transition properties, we have studied the anharmonic phonon spectra of bulk CuTe within the stochastic self-consistent harmonic approximation (SSCHA).[6] In particular, by using the exchange interaction via semi-local functionals in the force calculation, we have determined the nature and the temperature of the CDW transition.[7]

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