Abstract:
Thermoelectrics provides a means to harvest energy sustainably from the environment and also plays an important role in materials science. Such environmentally friendly energy conversion sources are considered to be promising for supplementing future global energy demands. In recent years, low dimensionality (one-dimensional and two-dimensional) has opened up new routes to achieve high efficiency thermoelectric devices. High mobility two-dimensional (2D) transition metal dichalcogenides semiconductors represent a new class of thermoelectric materials due to their enhanced density of states of confined carriers, as well as their large effective masses and valley degeneracies.

In most cases, the Seebeck coefficient is determined by a normal energy-dependent electronic density of states near the Fermi level and the charge carrier type (electrons or holes). Thus in previous studies, only a negative Seebeck coefficient due to conduction electrons was observed in MoS2 based devices. In this study, we observe for the first time, a positive Seebeck coefficient in n-doped six-layer MoS2 at temperatures below ~70K, which indicates that the Seebeck effect originates from the change in energy dependence of the charge-carrier relaxation times. The measured mobility undergoes a concomitant change in the slope at the same temperature, which corroborates a change in the relaxation time as a function of temperature and results in a sizable positive addition to the Seebeck coefficient. At low temperatures, we observe a large positive Seebeck (~ 1.5 mV/K at 50K). This new finding advances the study of thermoelectric physics in 2D materials and demonstrates a new avenue for superior thermoelectric performance by tuning the energy-dependent relaxation time.

Abstract:
This talk will present a study of the effects of realistic electron-electron interactions in graphene at half-filling. In this study we use projective quantum Monte Carlo simulations of electrons living on the honeycomb lattice and interacting through an effective Coulomb potential. We compute the antiferromagnetic ordering, the renormalized Fermi velocity and the quasiparticle residue as a function of the strength of the short- and the long-range components of the effective Coulomb potential. We find that the short-range part of the potential is more efficient in driving the semi-metal to Mott insulator transition than the long-range part. We then argue that isotropic strain may bring graphene close to such phase transition. This transition is consistent with the Gross-Neveu-Yukawa critical theory. Far from the critical point, the Fermi velocity renormalization is dominated by the long-range part of the interaction, being compatible with the predictions from perturbative theory for massless Dirac fermions interacting through a bare Coulomb potential. In contrast, close to the Mott insulator transition, the Fermi velocity behavior is modified by a competition between spin density wave and charge density wave fluctuations. Interestingly, real graphene samples are generally in between these two limits. Since finite system sizes restrict the QMC results to large momentum scales, we perform a phenomenological reconstruction of the renormalization group flow of the Fermi velocity, so that we can make predictions testable against recent experimental observations. Finally, we look at the quasi-particle residue, which is found to interpolate between unity and zero as we move from the weakly interacting regime into the close vicinity of the phase transition.