Emergence of correlated states in 2D crystal with ultraflat bands: multilayer graphene and single layer 1T-$NbSe_2$

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Abstract: The occurrence of strongly correlated states requires the dominance of the electron-electron interaction over the electronic kinetic energy. In the case of 3d transition metal oxides or high-Tc superconductors, Mott insulating and magnetic states are stabilized via the strong localization of electrons in 3d orbitals. Recently, it has been shown that a new class of strongly correlated systems can be achieved in ultraflat edge-states or surface bands having very small Fermi velocities, as it happens in twisted bilayer graphene[1,2]. In this talk, I will show my recent effort in understanding exchange and correlation effects in flat-band systems. In the first part of the talk I will consider multilayer graphene with rhombohedral stacking. I will first show how to identify the Raman signature of multilayer ABC stacked graphene[3]. Then I will demonstrate that comparison between ARPES data and first principles electronic structure calculations on flakes of approximately 14 layers reveals the existence of flat electronic bands and a gapped magnetic state[4,5]. Finally, by simulating the effect of the electric field on the sample in a field effect configuration, I will show that a perfect half-metallic behavior can be induced in the ABC multilayers[6]. In the second part of the talk I will present the study of the structural, electronic and vibrational properties of the recently-synthesized single-layer 1T-$NbSe_2$ from first principles. Within the generalized gradient approximation, the 1T polytype is highly unstable with respect to the 2H. Inclusion of correlation effects via the DFT+U method improves the stability of the 1T phase, explaining its detection in experiments. A charge density wave occurs with a sqrt(13)xsqrt(13)R30 periodicity, in

agreement with STM data. At U=0, the David-star reconstruction displays a flat band below the Fermi level with a marked dz2-r2 orbital character of the central Nb. The Hubbard interaction induces a spin 1/2 Jahn-Teller Mott insulating state. Magnetism distorts the lattice around the central Nb atom in the star, reduces the hybridization between the central Nb dz2-r2 orbital and the neighboring Se p-states and lifts in energy the empty dz2-r2 flat band becoming non-bonding. This cooperative Jahn-Teller and correlation effect is responsible for the gap opening[7].

References:

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