Mesoscopic Modeling of 2D Materials

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Abstract

Detailed understanding of the electronic, transport and optical properties of 2D materials requires the study of systems crossing over from microscopic to mesoscopic. New quantum phenomena emerge in mesoscopic structures, such as interference effects, quantum confinement effects, and charging effects. The ab initio calculations, including density functional theory and its extensions such as the GW-approximation and time-dependent DFT, are powerful tools for systems up to thousands of atoms, but become too computationally expensive and time-consuming with increasing system size. For structures with scales larger than 100 nanometers, such approaches are unfeasible.

Tight-binding propagation methods (TBPMs) [1-5] are a set of new numerical methods for the modeling of systems range from microscopic to mesoscopic level. TBPMs are based on the wave propagation of electron according to the time-dependent Schrödinger equation, and applied in the calculations of various properties, including but not limited to density of states, quasieigenstates, static and dynamic (optical) conductivity, polarization function, dielectric function, energy loss function, plasmon damping rate, diffusion coefficients, mean free path, localization length, electron velocity and mobility, magnetic susceptibility, and tunneling probability. The magnetic field is introduced by means of the Peierls substitution and the effect of electron-electron interaction is considered within the random phase approximation. The computational effort of the calculation increases only linearly with the system size, which makes the methods extremely powerful in the mesoscopic simulation with detailed atomic structure, especially in systems where the translational invariance does not hold, for example, the presence of random or correlated disorders or structures.

In this talk, I will first give a brief introduction of the numerical methods, and then show their applications together with our very recent progresses in the study of 2D materials, such as the reduced optical gap in fluorographene due to various structure disorders [6] (Figure 1), many-body enhancement of insulating states at the additional Dirac points in graphene-*h*BN heterostructures [7] (Figure 2), effects of disorder in the electronic and optical properties of semiconducting black phosphorus [8-9] and transition metal dichalcogenides [10], a new tight-binding model parametrization for black phosphorus with an arbitrary number of layers [11], quantum Hall effects in biased black phosphorus [12], and conductance fluctuations in novel 2D fractals [13]. I will also show how to combine the TBPMs with other well-known numerical methods such as DFT-GW and molecular dynamics, and discuss briefly possible extension of TBPMs to the study of many-body problem.

References

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Figures

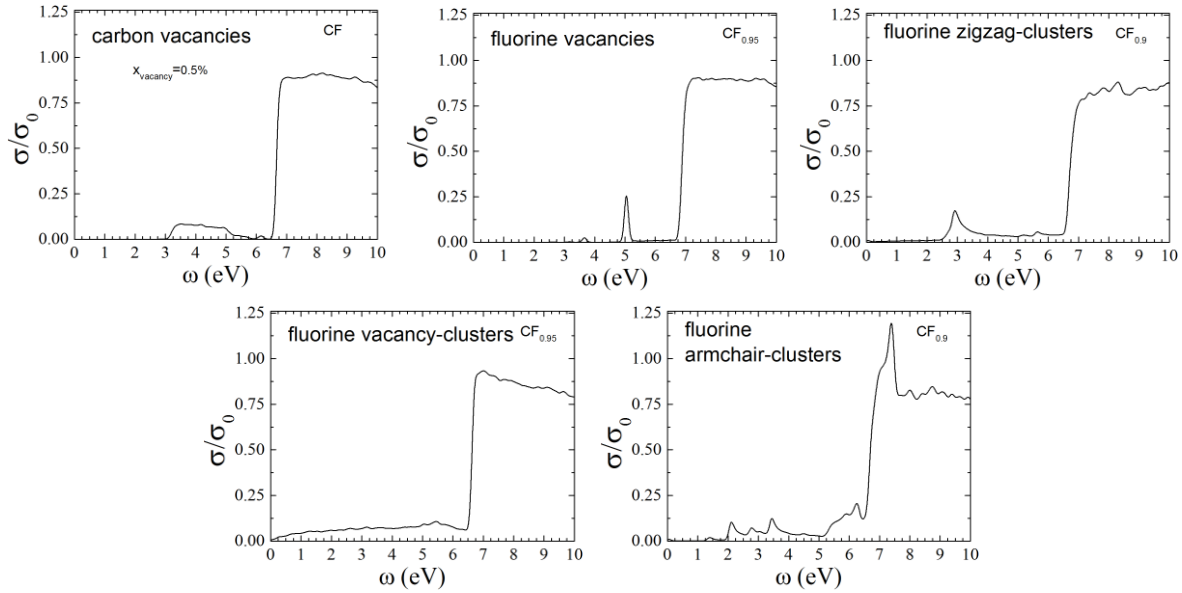

Figure 1. Optical conductivity of fluorographene (CF) with various structure disorders.

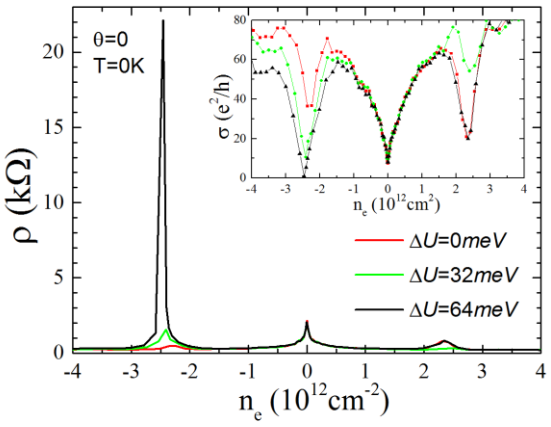

Figure 2. Transport property of graphene on top of *h*BN. The additional Dirac point on the hole side becomes insulating when considering the many-body enhancement of the local gap between the sublattices, which is clarified by ΔU. The numerical results reproduce the transport measurements of graphene/*h*BN heterostructure performed by L. A. Ponomarenko, *et al*, in Nature **497**, 594 (2013).