RECENT ACHIEVEMENTS OF DENSITY FUNCTIONAL THEORY IN ELECTRONIC SYSTEMS

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The main feature of the electronic systems in atoms, molecules and solids is that external potential as well as mutual interaction between electrons has the form of Coulomb potential. In such a case, the knowledge of the one-particle density determines not only the ground state energy of the electronic system but also the full Hamiltonian of the systems. Therefore, the very special properties of the Coulomb density allow for formulation of an exact time-independent density functional theory (DFT) of ground and excited states of Coulomb systems [1]. Since the Kohn-Sham theory is the most frequently implemented realization of the DFT and commonly used in condensed matter problems, I will also discuss the Kohn-Sham theory for excited states of Coulomb systems [2] based on energy stationary principle introduced by Görling [3] for an universal functional of the density and demonstrate the derivation of the single particle Kohn-Sham equations.

In recent years, the reliable DFT calculations have become a prerequisite for design of novel materials with required functionalities. The need for high accuracy predictions has induced very strong activity for search for better approximations to the exchange and correlation functionals. I will illustrate this trend by discussing the role of DFT calculations for prediction of the nanostructured gas-adsorbent materials (GAMs) [4]. These are the corner-stones of potentially revolutionary advancements in critical and fast growing technological fields such as molecular sensing, energy storage and harvesting, and environmental and sustainability engineering. Among these issues are hydrogen storage and carbon capture and sequestration challenges. The standard DFT approximations present some well-known limitations in describing gas-adsorption phenomena occurring in low-coordinated atomic environments. The two main problems in the standard DFT approximations are: (i) spurious self-interaction, and (ii) impossibility to record for long-range dispersive van der Waals forces. It turns out that for fairly good description of the adsorption processes DFT exchange-correlation functionals employed in modeling of GAM must incorporate features correcting somehow for standard self-interaction errors and simultaneously reproduce dispersion forces. The recent proposals for such functionals will be reviewed. The issue of vdW forces will be also exemplified with our own results for hydrogenated and fluorinated graphene on metallic and insulating substrates.

Finally, I would like to stress the role the DFT has played for development of modern materials science and point out areas of physico-chemistry for which the further progress without DFT is unthinkable.

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