DCP Symposium for the March 2016 Meeting of the APS in Baltimore

Recent Advances in Density Functional Theory and Applications in Chemical Physics

Organizers

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Description

Density Functional Theory (DFT), in both its ground-state and time-dependent (TD) flavors, is an exact reformulation of the quantum mechanics of many-body systems. Used in more than 10,000 papers annually, DFT provides an unprecedented balance of accuracy and efficiency for electronic structure and response calculations in molecules, clusters, and solids. DFT is often the only computationally feasible, quantum mechanical approach to some of the most interesting and topical problems in chemical physics today: including catalysis, stacking interactions in DNA, the design of solar cells, many aspects of photodynamics, molecular, ionic, and electronic transport, and time-resolved spectroscopies. There are however many problems for which there is room for improvement in the currently used functional approximations and formulations of DFT; these applications include strongly correlated and multireference systems, transition metal chemistry, dynamics far from equilibrium, and globally accurate potential energy surfaces, and there is significant on-going progress to address these challenges. Even in situations where approximate density functionals tend to work well, more needs to be done to understand why and to improve the approximations. And the effort to find universal methods that work well in all the areas of interest, as required for the most complex applications, also continues. This symposium highlights some of the recent advances in both theory development and applications. The symposium is open to contributed talks to complement the invited talks and to broaden the scope.

Invited speakers (all confirmed)

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