Density Functional Theory for Chemical Physics

Density Functional Theory, in both its ground-state and time-dependent (TD) flavors, is an exact reformulation of the non-relativistic quantum mechanics of many-body systems. Used in more than 10,000 papers per year, DFT provides an unprecedented balance of accuracy and efficiency for electronic structure 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: from stacking interactions in DNA, to the design of solar cell candidates, to photodynamics and molecular transport.

There are however many problems for which DFT performs notoriously poorly. Several open questions that will be addressed are:

- **Orbital-free DFT**: A dream or a reliable reality?
- **Weak molecular interactions**: how reliable and universal are the functionals for hydrogen bonds? for van der Waal's?
- **Strongly-correlated systems**: Can we dissociate H_2 and H_2^+ correctly?
- **Energy applications**: What are the realistic prospects for accurate modeling of energy applications? What are the most crucial aspects of the approximate functionals for this purpose?
- **Excitons**: Can they be described in TDDFT?
- **Potential-energy surfaces**: How can we make potential energy surfaces globally accurate enough to be used confidently for phenomena such as photo-induced dynamics in biomolecules?
- **Beyond Born-Oppenheimer**: How should we correctly account for ionic motion coupled to electron dynamics?
- **Strong-field physics**: How useful is time-dependent DFT for attosecond control, multiple-ionization, charge-resonance enhanced ionization…?

This symposium will highlight recent advances in both theory development and applications.

<u>Symposium Organizers:</u>

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