ID: 1.4.1a

Title: Approaches for the simulation of open quantum systems and quantum computation with time-dependent density functional theory

Name: Aspuru-Guzik, Alan

Affiliation: Harvard University

Every quantum system interacts with its environment to a certain degree, and therefore, the simulation of molecular systems as energy-conserving, closed quantum mechanical objects is an idealization. Historically, most of the molecular electronic structure approaches to date have concentrated on the simulation of time-independent or time-dependent systems that do not interact with quantum environments, and therefore, cannot exhibit relaxation or dissipation dynamics following an approximate equation of motion. We recently developed a framework for simulating the time-evolution of an open quantum system using an auxiliary closed Kohn-Sham system evolving under a unitary evolution. We have also explored a linear-response time-dependent density functional theory (TDDFT) approach which incorporated bath effects via a Gorling-Levy type perturbative formalism. The former approach is ambitious but strongly simplifying, and the latter is more systematic but also more costly. Both give access to finite excited state lifetimes not accessible in usual quantum chemistry calculations. We have made progress in developing relaxation and dissipation functionals. I will describe these approaches. I will finish by describing a surprising set of new proofs for TDDFT in the context of universal quantum computation.