“Large Scale Studies of Many Electron Systems using Time Dependent Stochastic Density Function Theory”

Time dependent density function theory (TDDFT) can be a powerful method for determining the electronic energy, electronic structure, and electron dynamics of a many electron system. TDDFT is highly versatile, but its scales poorly with the size of the system. This prevents TDDFT from being implemented to large systems containing thousands of electrons. The ability to study these systems could provide important information, which could be used to create new theories for phenomena which couldn’t be explain otherwise. In an effort to reduce the cost of TDDFT, we develop a method in which the electronic densities of smaller fragments are determined by Kohn-Sham density function theory (DFT). These fragments are then embedded into our time dependent stochastic DFT (TDsDFT). This new method reduces the cost of TDDFT, while still retaining its accuracy. This allows us to study larger systems, which would otherwise be too costly with the conventional method. I will discuss two such systems in my presentation.

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