

Time-Dependent Exchange-Correlation Potentials for Non-Perturbative Dynamics

Neepta T. Maitra

Hunter College and the Graduate Center of the City University of New York, 695 Park Avenue,
New York, NY 10065

Time-Dependent Density Functional Theory is increasingly used beyond linear-response, involving applications where the electronic system is driven far from its ground-state, such is the case in photovoltaic device operation, attosecond control of electronic and ionic motion, and photo-induced processes generally. Although it has produced useful results in several topical cases, its reliability is questionable due to the adiabatic approximations made for the exchange-correlation potential. In this talk I show some of our recent work exploring exact features of the time-dependent exchange-correlation potential that are necessary to yield accurate dynamics, and discuss approaches to develop new functionals going beyond the adiabatic approximation.