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Title:

Maximally-Localized Wannier Function Propagation in RT-TDDFT

Abstract:

We discuss our recent work on propagating time-dependent maximally-localized Wannier functions (TD-MLWFs) for studying electronic excitation and dynamics in complex systems using real-time time-dependent density functional theory (RT-TDDFT). In particular, our implementation in the massively parallel Qb@ll code is discussed, and we present its application to studying non-equilibrium energy transfer excitation in liquid water and solvated DNA under proton irradiation. We further discuss utilization of TD-MLWFs to study plasmon excitation transfer at heterogenous interfaces and how hybrid exchange-correlation (XC) functionals can be implemented efficiently using TD-MLWFs.