**TDDFT Study of Electron Scattering Processes**

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Time-dependent density functional theory (TDDFT) is the most widely used first principles approach to study real-time many-electron dynamics. TDDFT with approximate exchange-correlation (XC) potentilas has been successfully applied to interpret and predict electron dynamics in a range of situations. Recently, it has been applied to the real-time nonperturbative calculations of electron wave packet scattering from atomic layer materials [1-5].

However, it is known that TDDFT with approximate XC potentials fails to even qualitatively reproduce the true dynamics in some applications to nonlinear time-resolved dynamics. In this study [6, 7], we address the question how accurate TDDFT with the currently available approximate XC potentials is for electron scattering. To this end, we have studied model systems of electron-H and electron-He+ scattering that can be exactly solved numerically.

We have identified peak and valley structures in the exact XC potential that are crucial for accurately capturing time-resolved dynamics of electron scattering [6, 7]. Approximate functionals used today miss these structures and consequently underestimate the scattering probability. The dynamics can vary significantly depending on the choice of the initial Kohn-Sham state. A recently propsed nonadiabatic approximation is shown to correctly capture the approach of the electron to the target when the initial Kohn-Sham state is chosen judiciously, and it is more accurate than standard adiabatic functionals but ultimately fails to accurately capture reflection. These results may explain the underestimation of scattering probabilities in some recent studies on molecules and surfaces.

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