

Real-time implementation of TDDFT

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K. Yabana and I have developed a real-time, real-space method to calculate optical responses in the time-dependent density-functional theory. The computational effort and the memory requirements for the method scale quadratically with system size for finite systems, which makes the method advantageous for large molecules or clusters. I will show applications to the collective electronic excitations of metallic clusters, absorption spectra of conjugated carbon systems, and the optical activity of chiral molecules. I will also show a gauge field extension that allows the method to be applied to the dielectric function of infinite crystalline systems, with metallic lithium and diamond as examples.