

Real-Time TDDFT Selective Range Spectroscopy with Applications

Ivan Williams, Eric Polizzi

Department of Electrical and Computer Engineering,
University of Massachusetts, Amherst

We demonstrate the ability to simulate targeted excitations of atomistic systems using our real-time TDDFT-based simulation framework NESSIE. Traditional approach for extracting spectra through real-time TDDFT involves excitation of all frequencies via impulse. For example, small time steps (tenths of attoseconds) are required to obtain spectral responses in the X-ray regime. In order to accurately compute the spectral response of the impulse the fourier transform of the dipole oscillations must be computed over several femtoseconds. By exciting the system with a modulated sinc pulse between the frequencies of interest we are able to obtain a spectral response with far more precision in a significantly shorter timeframe than competing implementations. Additionally with the inclusion of 'soft' molecular dynamics we aim at resolving vibrational spectra as we can confine excitations to the mid-IR regime.