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Applying state-of-the-art signal processing to time-dependent density functional theory JACOB SANDERS, XAVIER ANDRADE, ALAN ASPURU-GUZIK, Harvard University Department of Chemistry and Chemical Biology — Real-time time-dependent density functional theory (TDDFT) is a computationally efficient method that can be used to calculate optical absorption spectra, circular dichroism spectra, and other properties including non-linear ones. These properties are often obtained via time-propagation methods, and a discrete Fourier transform is used to convert from the time domain to the frequency domain. However, a Fourier transform requires long time propagations to resolve spectra, especially if they contain closely-spaced frequencies. Instead, we apply a state-of-the-art signal processing technique known as compressed sensing to the spectral analysis of electron dynamics. Compared to a Fourier transform, compressed sensing provides higher-resolution absorption spectra with shorter propagation times. In the systems we study, the method requires about 80% less time series data to obtain comparable frequency resolution, thus reducing total computational cost by approximately a factor of five. By combining the computational efficiency and parallelizability of real-time TDDFT for large systems with the dramatic reduction in simulation time enabled by compressed sensing, we increase the feasibility of studying electron dynamics in large biological molecules and organic photovoltaics.

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