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Verifying TDDFT with Ultrahigh Resolution X-ray Thomson Scattering Measurements

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The dynamic structure factor (DSF) of a system provides a wealth of information on its properties, such as its temperature, density and on electron correlations. The state-of-the-art approach to calculating the DSF is using time-dependent density functional theory (TDDFT), which provides an in-principle exact calculation of the full electronic response of the system in an ionic environment. The DSF can also be directly measured in experiment via x-ray Thomson scattering (XRTS), but it is convolved with the source-and-instrument function (SIF) of the setup. The rigorous benchmarking of TDDFT with experiment is challenging due to (a) the need to precisely know experimental conditions, and (b) the SIF needs to be carefully handled as it otherwise obscures features in the DSF. Here, we present results from a novel ultrahigh resolution setup at the European XFEL. The SIF of this setup is sufficiently narrow that its broadening of the measured DSF is negligible. We have used this setup to benchmark TDDFT-predicted DSFs in ambient conditions for simple metallic Al and single crystal semiconducting Si. Once the experimental geometry is accounted for, we find TDDFT produces accurate DSFs over a range of scattering vectors. We conclude by considering applications of ultrahigh resolution spectroscopy to broader experimental scenarios.

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