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Resonant X-ray spectroscopy of selenophene with hard-X-ray pulses

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Due to their short wavelengths, hard-X-ray FEL pulses are sensitive to spatial variations within the size of the molecule. They can thus monitor the evolution of the molecular charge and current densities. This is shown for the resonant X-ray sum-frequency-generation (XSFG) signal of aligned selenophene molecules [1]. A wavepacket of valence-excited states, initiated by an XUV pump pulse, is monitored by 12-keV X-ray probe pulses resonant to the Se core states for variable time delays. The associated wavelength of the X-ray probe, $\lambda \sim 1 \text{ \AA}$, is comparable to the molecular size. By varying the propagation direction of hard-X-ray pulses, we predict observable changes in the XSFG signal, which can be attributed to the spatial dependence of the transition current densities in the molecule.

We further apply related time- and frequency-resolved X-ray Raman signals to monitor nonadiabatic molecular dynamics. By taking advantage of the correlations between the spectral components of the field, we show that high joint spectral and temporal resolutions can be achieved, without requiring phase control [2]. The approach can thus be applied with existing stochastic SASE FEL pulses.

[1] S. M. Cavaletto and S. Mukamel, J. Chem. Theory Comput. (2020),

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[2] S. M. Cavaletto, D. Keefer, and S. Mukamel, manuscript submitted (2020).

Primary author: CAVALETTO, Stefano (University of California, Irvine)

Co-authors: KEEFER, Daniel (University of California, Irvine); MUKAMEL, Shaul (University of California, Irvine)

Presenter: CAVALETTO, Stefano (University of California, Irvine)

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