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Attosecond Molecular-Frame Angular Distribution of Electronic Coherence[1] SHUNGO MIYABE, RIKEN, R. LUCCHESE, Texas A&M University, C. W. MCCURDY, Lawrence Berkeley National Laboratory, University of California, Davis — Using *ab initio* electron-ion scattering calculations, it is demonstrated that for a molecule, oriented in space and excited by an attosecond pulse, the degree of electronic coherence left in the ion depends sensitively not only on the orientation of the electric field polarization vector in the molecular frame, but also on the details of the angular distribution in the molecular-frame of electrons ejected in different ionization channels. Accurate modeling of the degree of coherence induced by attosecond ionization in the molecular ion can require a coupled-channel electron-ion scattering wavefunction, which takes interactions of various ionization channels into account and also the inclusion of electron correlation in the wavefunctions of the ionic states, both of which make a notable difference the computed results presented here for the water and glycine molecules. Numerical simulations reported here are based on one-photon single ionization amplitudes calculated using the complex-Kohn variational method, and the amount of coherence in the ion is expressed in terms of the N-electron reduced density matrix of the full $(N+1)$-electron system of the ion plus ionized electron.

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