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Theoretical predictions of the impact of nuclear dynamics and environment on core-level spectra of organic molecules DAVID PRENDERGAST, Molecular Foundry, Lawrence Berkeley National Laboratory, CRAIG SCHWARTZ, JANEL UEJIO, RICHARD SAYKALLY, Chemical Sciences Division, Lawrence Berkeley National Laboratory — Core-level spectroscopy provides an element-specific probe of local electronic structure and bonding, but linking details of atomic structure to measured spectra relies heavily on accurate theoretical interpretation. We present first principles simulations of the x-ray absorption of a range of organic molecules both in isolation and aqueous solvation, highlighting the spectral impact of internal nuclear motion as well as solvent interactions. Our approach uses density functional theory with explicit inclusion of the core-level excited state within a plane-wave supercell framework. Nuclear degrees of freedom are sampled using various molecular dynamics techniques. We indicate specific cases for molecules in their vibrational ground state at experimental conditions, where nuclear quantum effects must be included. Prepared by LBNL under Contract DE-AC02-05CH11231.

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