Abstract Submitted
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Validity of the static-exchange approximation for inner-shell photoionization of polyatomic molecules[1] C. MARANTE, Lawrence Berkeley National Lab, L. GREENMAN, Kansas State University, C. S. TREVISAN, CSU Maritime Academy, T. N. RESCIGNO, Lawrence Berkeley National Lab, C. W. MCCURDY, UC, Davis and Lawrence Berkeley National Lab, R. R. LUCCHESE, Lawrence Berkeley National Lab, AMOP TEAM — The single-channel static-exchange approximation, which completely ignores correlation between the continuum and molecular ion electrons, is demonstrated to fail seriously for molecules with symmetry equivalent atoms whose core shells are being ionized when delocalized symmetry orbitals are used. We present cross sections and molecular frame photoelectron angular dependences (MFPADs) with both uncoupled and coupled ionization channels together with an analysis of the validity of the single-channel approximation to explain why and how it breaks down and the degree of channel coupling required to recover an accurate description of the physics of inner-shell photoionization. When localized core hole wave functions are used, the photoionization calculations as a single-channel computations then give accurate results, when the MFPADs with the hole in the different symmetry equivalent locations are summed. A grid-based variational method, relying on a central grid and off-center subgrids on the nuclear positions is described, that makes such calculations possible on larger systems.

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