

# **Cross sections and photoelectron angular distributions in photodetachment from negative ions using EOM-CCSD Dyson orbitals**

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Experimental photoelectron angular distributions (PADs) contain information about the excited states of less stable compounds and their dissociation mechanism, but the interpretation of the results is difficult for molecules with complex electronic structure, e.g. NO dimer, CS<sub>2</sub> photodissociation. Ionization cross-sections and PADs can be calculated from the corresponding electronic transition dipole matrix elements.

The wavefunction of the leaving electron is given by Dyson orbitals, which are the overlap between an  $N$  electron molecular wavefunction and the  $N-1/N+1$  electron wavefunction of the corresponding cation/anion. Our implementation of the Dyson orbitals calculation within the high level ab initio EOM-IP/EA-CCSD method, allows the calculation of these terms for the ionization of electronically excited states and open-shell species, when correlation effects become important. As a first approximation, the states of the ionized electron are described by plane waves expressed in the bases of spherical waves,  $|E, l, m\rangle$ .

Currently, the calculation of photodetachment cross-sections and anisotropies is benchmarked on atoms, and small molecules. Calculated PADs for NO dimer photodissociation allow qualitative comparison with experimental distributions. In the case of larger, anisotropic molecules, the development of better approximations for the description of the ionized electron is necessary.