EOM-CCSD absorption and emission spectra between arbitrary states

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Plasma gas reactions involve intricate processes, and optical emission spectroscopy (OES) stands out as a well-established tool to unravel the underlying physics of plasma phenomena. OES spectra observation facilitates the identification and quantification of molecules (as well as their fragments) present in plasma. The accurate characterization of gas molecules is pivotal for this purpose, and quantum chemical methods play a crucial role by providing transition energies and rates through various excited state methodologies. Among these, coupled-cluster theory emerges as a highly reliable option.

In our recent work, we have implemented the higher-order transition moment (beyond dipole) within the equation-of-motion coupled-cluster with singles and doubles (EOM-CCSD) level of theory. This implementation allows for accurate descriptions of transitions requiring higher-order moments, such as quadrupole moments. Notably, K pre-edge transitions fall into this category, and the inclusion of higher-order moments aligns well with experimental observations.

This study delves into the extension of transition moments between any two excited states, expanding our understanding of electronic transitions in plasma gases. We present several examples focusing on prominent plasma gases, including N_2, O_2, and CF_4. Additionally, the effects of surrounding noble gases (He and Ar) are considered to account for environmental influences on the electronic transitions within the plasma.