Probing the Open-Shell Character of Molecules via X-Ray Absorption Spectroscopy

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X-ray absorption spectroscopy (XAS) enables the characterization of reaction dynamics and chemical structure in an element-specific way. Theoretical simulations are of critical support in the analysis of XAS spectra, hence a significant endeavor has been made to develop new methods to compute core-excited states. There are several established methods that accurately simulate XAS, however, most are based on a single-reference formalism and may fail to describe molecular systems with open-shell character. Our recently proposed GASSCF-MR-DSRG method combines a generalized-active-space self-consistent-field (GASSCF) treatment of static correlation with dynamical correlation corrections from the driven similarity renormalization group (DSRG). In this study we compute the core-excited states of benzyne diradicals, and investigate how the multireference character of these molecules can be reflected by the splitting and the intensity ratio between transitions to frontier natural orbitals in their XAS spectra.