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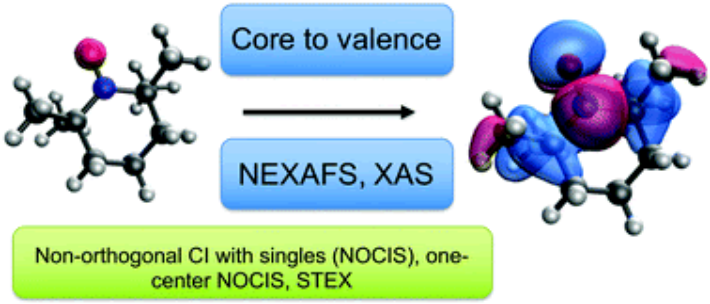
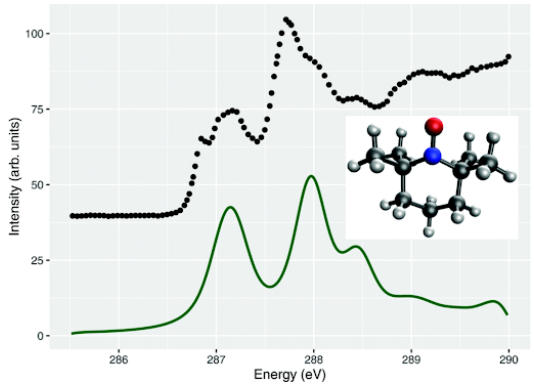
Non-Orthogonal Configuration Interaction with Single Substitutions (NOCIS) for Core-Excited States

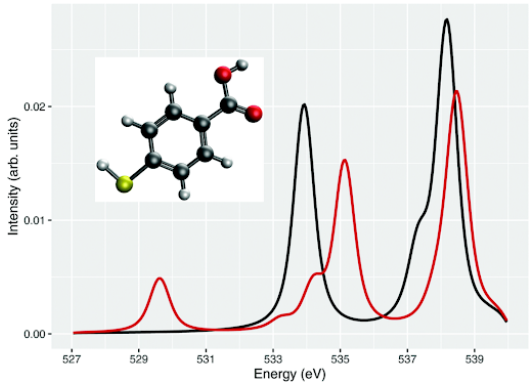


Simulation of X-ray absorption spectra (XAS) by NOCIS:

- NOCIS is a non-orthogonal configuration interaction (NOCI) method applied to core-excited states. In the case of a single core-hole reference, it is identical to the static exchange (STEX) method.
- In NOCIS, orbital relaxation is treated via a ROHF calculation and static correlation between the non-orthogonal core-hole configurations is included through CI. Dynamic correlation is absent in NOCI, but may be included through perturbation.
- NOCIS is designed as a black-box theory: it includes a precisely defined set of determinants.
- NOCIS ansatz is spin-pure, size-consistent, and obeys spatial symmetry.
- NOCIS can deliver accurate core-excitation energies, comparable to the high-level methods such as ADC and EOM-CC, but at a much lower computational scaling.
- Costs can be further reduced by one-center (1C)-NOCIS approximation.



(a) 1C-NOCIS and experimental XAS for the carbon edge of (2,2,6,6-tetramethylpiperidin-1-yl)oxyl



(b) 1C-NOCIS spectra for singlet (black) and triplet (red) 4-mercaptobenzoic acid

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