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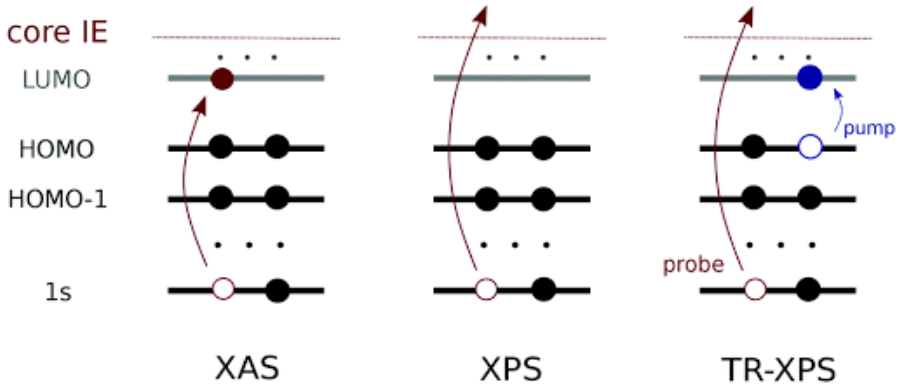
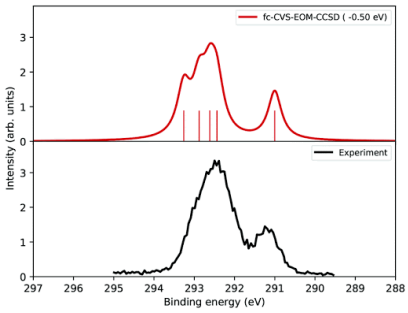
X-ray Photoelectron Spectroscopy of Ground and Excited States

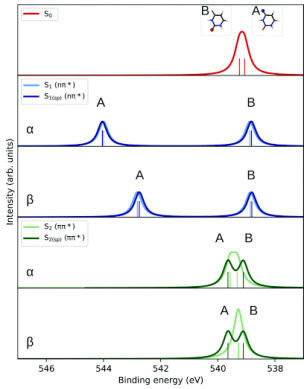


Simulation of X-ray photoelectron spectra (XPS) by fc-CVS-EOM-IP-CC (frozen-core core-valence-separation equation-of-motion coupled-cluster method for ionization potentials):

- EOM-IP-CC: the ground state is treated at the CC level and the ionized states are accessed by applying an ionization operator to the ground-state wavefunction. Excited states are accessed by MOM.
- FC approximation: omitting core-core and core-valence correlation in the ground state.
- CVS scheme: the EOM states are represented in a restricted Fock space spanned the many-electron determinants with at least one occupied core orbital index.



(a) Carbon K-edge XPS of ground-state adenine



(b) Oxygen K-edge XPS of electronically excited uracil

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