Insight Into The X-Ray Absorption Spectra of Cu-Porphyrazines From Electronic Structure Theory

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Abstract

Transition metal porphyrazines are a widely used class of compounds with applications in catalysis, organic solar cells, photodynamic therapy and nonlinear optics. The most prominent members of that family of compounds are metallophtalocyanines that have been subject of numerous spectroscopic and theoretical studies. In this work, the electronic structure and X-ray absorption characteristics of three Cu-porphyrazine derivatives are investigated by means of modern electronic structure theory. More precisely, the experimentally observed N K-edge and Cu L-edge features are presented and reproduced by time-dependent density functional theory, restricted open-shell configuration interaction and a restricted active space approach. Where possible, the calculations are used to interpret the observed spectroscopic features in terms of electronic transitions and furthermore connect spectral differences to chemical variations. Part of the discussion of the computational results concerns the impact of various parameters and approximations that enter the calculations, e.g. the choice of active space.

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