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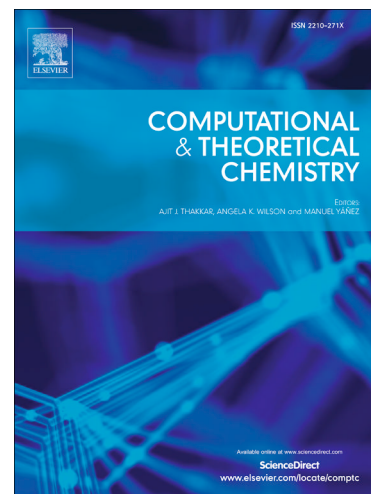
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Gang Sun, Xiang-Shuai Liu, E Lei, Chun-Guang Liu

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Theoretical Investigation on the Electronic Properties and UV-Vis Absorption Spectra of Expanded Porphyrin Mono-Cu(II) Complexes

Gang Sun ^{*,a}, Xiang-Shuai Liu ^a, E Lei ^a, Chun-Guang Liu ^b

^a*Chemistry and Biology Academy, Beihua University, Jilin 132013, China*

^b*College of Chemical Engineering, Northeast Dianli University, Jilin 132012, China*

*Corresponding author. E-mail: bhhxsg@163.com;

Tel: +86 043264602558; Fax: Tel: +86 043264602558

Abstract: The metalation chemistry of expanded porphyrins exhibits wide-ranging applications in numerous fields. In the work, we have investigated the electron spin density, charge transfer, frontier molecular orbitals and UV-Vis absorption spectra of four expanded porphyrin mono-Cu(II) complexes (Cu(II)@P, Cu(II)@HP, Cu(II)@OP and Cu(II)@d-OP) using density functional theory (DFT) method and time-dependent DFT. The results show that Cu(II)@HP has different electronic properties and absorption spectra compared with other complexes. What is more interesting is that the single electrons of Cu(II)@HP are not only distributed on the Cu atom and the four coordination N atoms, but also on the uncoordination conjugated pyrroles. However, the single electrons of other complexes are mainly distributed on the Cu atom and the four coordination N atoms. This phenomenon can be successfully explained by the specific mechanism of Cu(II)@HP unlike the Zn(II)@HP. Meanwhile, the calculated values of extended charge decomposition analysis indicate that beta electrons of Cu(II)@HP have more transfer, and its frontier molecular orbitals demonstrate greater involvement of Cu(II) ion compared

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