Abstract Submitted
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Essential factor for DFT predictions of relative energies in FePc: A Diffusion Monte Carlo study[1] TOM ICHIBHA, School of Information Science, JAIST, ZHUFENG HOU, National Institute of Materials Science, KENTA HONGO, RYO MAEZONO, School of Information Science, JAIST — The ground state of the isolated iron phthalocyanine (FePc) with D_{4h} symmetry is still unclear because the previous DFT works gave different predictions owing to their XC functionals. We applied CASSCF+DMC to evaluate the relative energies of the electric configurations reliably without XC functionals. A_{2g} configuration is predicted as the ground state, which is, we found, able to be justified by the recent spectroscopy for FePc gas. Furthermore, we considered why the DFTs give the different predictions. We compared several DFTs with DMC, which include different percentages of exact exchange, and we revealed short-range exchange is essential for the prediction. We identified the discrepancies being due to the assumptions made in the superposition model, which has also been employed in literature to explain the ground state of FePc molecule. Our orbital analysis shows that the assumptions are too simple to describe the proper stabilizing mechanism explained by the orbital shapes: Over-simplified symmetry assumptions as well as the ignorance of outer ligand structures cannot capture the stabilization [destabilization] of b_{2g} [e_g] orbitals, those actually realizes A_{2g} as the most stable state.

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