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A DMC study on FePc electronic state TOM ICHIBHA, KENTA HONGO, RYO MAEZONO, Japan Adv Inst of Sci and Tech — We performed fixed-node DMC calculations on an isolated FePc [Iron(II) Phthalocyanine] using CASSCF nodal surfaces, getting its ground state, $^3A_{2g}$ $[d^2_{z^2}d^2_{xz,yz}d^2_{xy}]$. Virial ratios for each state are achieved to be within 0.042% around 2.0. Recent studies [1] are proposing a mixed state with $^3E_g(b)$ and $^3B_{2g}$ as the ground state, while past ab-initio calculations [2] are predicting $^3A_{2g}$ or $^3E_g(a)$, giving still controversial arguments even within isolated/no-LS coupling model. Under D_{4h} ligand field parameter space, ($10D_q$, D_t, D_s), the state, $^3A_{2g}$, is reported to be possible as a ground state [3], while it is not when we restrict the space into 2-dim sub-space corresponding to more specified symmetry as in FePc with plane square alignment of neighboring N to Fe ('superposition model' [4]). Our optimized geometry also satisfies the same symmetry, and hence appears to be contradicting to the ligand theory[4]. [1] J. Fernández-Rodríguez *et al.*, Phys. Rev. B **91**, 214427 (2015). [2] K. Nakamura *et al.*, Phys. Rev. B **85**, 235129 (2012). [3] P.S. Miedema *et al.* , J. Phys.: Conf. Ser. **190** , 012143 (2009). [4] M.D. Kuzmin *et al.* , J. Chem. Phys. **138** , 244308 (2013).

Tom Ichibha
Japan Adv Inst of Sci and Tech

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