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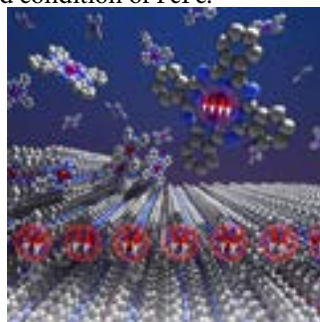
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Experimental and computational studies on the ground state of an isolated Fe(ii)-Phthalocyanine

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The electronic ground-state of the isolated Iron(II)Phthalocyanine (FePc) molecule is unknown. Previous experimental studies assigned the triplet as ground-state of FePc but they were performed either in gas phase at high temperature or in crystalline state. Using multi-reference CASPT2 and DMRG calculations we have shown that isolated FePc exhibits a quintet ground-state. This was further supported by Mössbauer spectroscopy and magnetic measurements of FePc in frozen non-polar chlorobenzene solvent which mimic the isolated condition of FePc.



Recent Publications

1. Lischka H, Nachtigallova D, Aquino AJA, Szalay PG, Plasser F, Machado FBC, Barbatti M (2018) Multireference Approaches for Excited States of Molecules. *Chem. Rev.* 118, 7293-7361.
2. de la Torre B, Svec M, Hapala P, Redondo J, Krejci O, Lo R, Manna D, Sarmah A, Nachtigallova D, Tucek J, Blonski P, Otyepka M, Zboril R, Hobza P, Jelinek P (2018) Non-covalent control of spin-state in metal-organic complex by positioning on N-doped graphene. *Nat. Comm.* 9, Article Number: 2831.
3. Kleinerann K, Nachtigallova D, de Vries M (2013) Excited state dynamics of DNA bases. *Int. Rev. Phys. Chem.* 32, 308-342.
4. Nachtigallová D, Antalík A, Rabindranath L, Sedlák R, Manna D, Tuček J, Ugolotti J, Veis L, Legeza O, Pittner J, Zbořil R, Hobza P (2018) An Isolated Molecule of Iron(II) Phthalocyanine Exhibits Quintet Ground-State: A Nexus between Theory and Experiment. *Chem. Eur. J.* 10.1002/chem.201804158.
5. Sedlak R, Eyrilmez SM, Hobza P, Nachtigallova D (2018) The role of the sigma-holes in stability of non-bonded chalcogenide ... benzene interactions: the ground and excited states *Phys. Chem. Chem. Phys.* 20, 299-306.

Biography

Dana Nachtigallová works as a senior researcher at the Institute of Organic Chemistry and Biochemistry of the CAS: Her current research interests focus on description of excited states of extended aromatic hydrocarbons and metallo-organic complex, simulations of nonadiabatic photodynamical processes, and modelling of noncovalent interactions of the excited state associates.

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