

Optimally Tuned Functional Methods as a Way of Improvement in the Description of Optical and Electronic Properties of Phthalocyanines Complexes

Authors: Tamires Lima Pereira, Luciano Almeida Leal, Luiz Antônio Ribeiro Junior,
Demétrio Antônio da Silva Filho

Address: University of Brasilia, Institute of Physics, 70.919-970, Brasilia, Brazil

Abstract: Organic compounds, such as metallophthalocyanines (MePc) have emerged as important candidates to be used as active materials in numerous applications. Several studies have addressed the impact of the position of the central metal atom relative to the organic cage of the phthalocyanine (Pc) and the possibility of exploiting it in numerous applications. We have employed the Density Functional Theory (DFT) to examine the structural, electronic and optical properties of MePc. Due to issues associated with multi-electron self-interaction errors of the conventional functionals, we use long-range corrected functionals, where the range separation parameter is tuned for each structure and the characteristic lengths ($1/\omega$) depend on the chemical nature and size of the system [1]. We analyze the first absorbing excited state energy for the various molecules investigated in this study. We can conclude that the energy of this state in both the molecules have values next comparing the values obtained with X-Ray geometries and the optimized geometry. We show the orbital energies of the highest three occupied orbitals and lowest three unoccupied molecular orbitals, both using the X-Ray and optimized geometries [2]. The HOMO→LUMO energy are very comparable in all the molecules studied. Another important result that this work presents is the optimization of ω parameter. Implementing the optimized ω on DFT methodologies, the results are improved on this job.

Key-words: Long Range Correction optimization, DFT, X-Ray geometries, Phthalocyanines

Support: This work has been supported by University of Brasilia, FAP-DF, CNPq and CAPES.

References:

[1] J-D. Chai, H-Gordon, *The Journal of Chemical Physics* 128 (2008) 84106.

[2] The Cambridge Crystallographic Data Centre (CCDC).