Characterization of charge transfer mechanisms in the molecular capacitor β-DiCC[Ni(dmit)$_2$] using TD-DFT methods

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Abstract

This study describes the charge transfer mechanisms in the redox equilibrium of the molecular capacitor β-DiCC[Ni(dmit)$_2$] by means of the DFT approach. Calculations on the DiCC and [Ni(dmit)$_2$] fragments show that the ionic form β-DiCC$^+$[Ni(dmit)$_2$]$^-$ is more stable than the neutral form β-DiCC^0[Ni(dmit)$_2$]^0 by 6.27 kcal/mol, in agreement with a spontaneously reversible redox (charge transfer) process, as proposed from the experiments. Time Dependent DFT calculations have been also performed for the excited states searching. A doublet excited state D_8, at 40.7 kcal/mol, has been found to be consistent with a photoinduced mechanism for the redox equilibrium within β-DiCC[Ni(dmit)$_2$]. A detailed description of the transitions, electronic structure, and charge transfer is also presented.

Keywords

Charge transfer, Molecular photoconductor, Reversible capacitor, TD-DFT.