DFT studies on coordination models for adsorption essays of Cu(II) and Ni(II) solutions in modified silica gel with iminodiacetic groups

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Research in functionalized inorganic supports faces special challenges regarding the inmobilization of organic chains and efficient computational methods for the quantum chemical modeling of coordination compounds. The silylant 3-cloropropyltriethoxysilyl (R1) was anchored over silica gel in anhydrous conditions, in order to react with diethyl Iminodiacetate (DIDA) to obtain modified silica gel (R2), which was hydrolized in basic conditions previously synthesized and characterized by S BET, TGA and FTIR spectroscopy to obtain iminodiacetic acid groups IDA to prepare an modified inorganic support (R3) that is able to get hands on metals from the first transition series such as copper and nickel. The obtained experimental values showed that the functionalized grade of R3 corresponds to 0.1598 mmol of the nitrogen indicated that the adsorbed Cu(II) or Ni(II) have the stoichiometry for both cation of 1:1. Based on this relation, the three different structures were proposed to carry out the computational studies using density functional theory (DFT) in its LDA and PW91 with the TZP slater type basis set. The primary coordination sphere of copper(II) or nickel (II) ion in R3 are optimized, structural parameters are calculated, vibrational bands are assigned and energy gaps of frontier orbital (HOMO-LUMO) have been calculated. The calculated results

reproduced the experimental data with good agreement. An energy decomposition analysis (EDA) of the different models proposed here was performed and suggest a 1:1 coordination form.

DFT

Modified inorganic support

Morokuma-Ziegler methodology

Silica gel