Configurational study of amino-functionalized silica surfaces: A Density Functional Theory modeling

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Abstract

Despite extensive studies of the amino-functionalized silica surfaces, a comprehensive investigation of the effects of configuration and hydrolysis of 3-aminopropyltriethoxysilan (APTES) molecules attached on silica has not been studied yet. Therefore, the methods of quantum mechanics were used for the study of configuration and hydrolysis forms of APTES molecules attached on the surface. For this purpose, five different categories based on the number of hydrolyzed ethoxy groups including 16 configurations were designed and analyzed by the density functional theory (DFT) method. The steric hindrance as an effective factor on the stability order was extracted from structural analysis. Other impressive parameters such as the effects of hydrogen bond and electron delocalization energy were obtained by using the atoms in molecules (AIM) and natural bond orbitals (NBO) theories. Consequently, it was found that the stability of configurations was attributed to steric effects, hydrogen bond numbers and electron delocalization energy. The maximum stability was achieved when at least two of these parameters cooperate with each other. Finally, we guessed that these surfaces could be used for immobilization of biomolecules such as enzymes and DNA.

Keywords: Amino-functionalized Silica, APTES, Hydrolyzed forms, DFT, AIM