Theoretical Study of the adsorption of Acetone onto SiO_2, TiO_2 and ZrO_2 Surfaces on the Basis of Ab Initio Hartree-Fock Calculations

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Abstract

An *ab-initio* quantum mechanical study of the adsorption of acetone on SiO_2, TiO_2 and ZrO_2 surfaces is reported. Ab-initio Hartree-Fock calculations have been carried out using 3-21G* and 6-31G(d) basis sets. Calculations show that Ac is weakly adsorbed on silica, resulting in the formation of two differently H-bonded species:

(i) Ac bound to a single terminal Si-OH, and

(ii) Ac bound to 2 Si-OH groups.

Calculations for TiO_2 and ZrO_2 show that stronger adsorption of acetone occurs on TiO_2 than on ZrO_2. Calculations also reveal that there is a direct relationship between the net cationic charge and the adsorption energy, as revealed by Mulliken population analysis. It is demonstrated that increasing the cationic net charge results in an increase of the Lewis acidity of the metal oxide. Calculations also show that TiO_2 possesses stronger Lewis acid sites than ZrO_2.

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