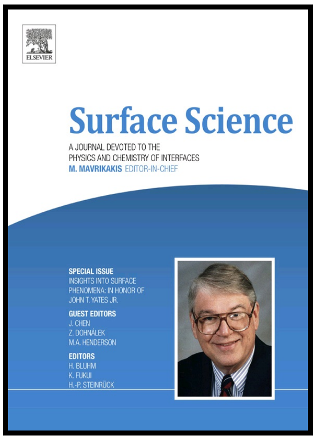

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Adsorption and dissociation of SO_3 on N-doped TiO_2 supported Au overlayers investigated by van der Waals corrected DFT

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Abstract

We present a density functional theory (DFT) study of the reactivity towards SO_3 adsorption and dissociation over the TiO_2 supported Au overlayers. We model different adsorption configurations of SO_3 on the considered structures. For all adsorption systems, we find that the interaction of SO_3 molecule with the surfaces of Au atoms is strongly favored. On the TiO_2 supported Au overlayer, SO_3 also dissociated into SO_2 and adsorbed atomic oxygen. The atomic oxygen binds directly to the Au atoms. The structural properties are explained in terms of the bond lengths, bond angles and adsorption energies. The electronic structure of the system and Mulliken population analysis were also studied for the discussion of results. The results indicate that the SO_3 interaction with N-doped TiO_2-supported Au overlayer is more favorable in energy than the interaction with undoped one, suggesting the increased sensing capability of N-doped TiO_2-supported Au towards detection of SO_3 molecule. The oxygen atoms of the SO_3 molecule bind to the Au and Ti atoms of the TiO_2 supported Au overlayer in a bridge geometry. The significant overlaps in the PDOSs of the Au and oxygen atoms of the SO_3 molecule, as well as titanium and oxygen atoms indicate the formation of chemical bonds between these atoms. Our DFT study therefore provides a theoretical basis for why the reactivity of SO_3 molecule with N-doped TiO_2 supported Au overlayer may increase, thus being a helpful procedure in the development of efficient sensor devices for SO_3 detection.

Keywords: Density Functional Theory; TiO_2; SO_3; TiO_2-supported Au overlayers; Adsorption