عنوان مقاله:

Adsorption of SO۲ and NO۲ on ZrO۲ (۱۱۰) Surface: Density Functional Theory and Molecular Dynamic Simulation Studies

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خلاصه مقاله:

In order to save the environment, there is an urgent need for control measures due to the rapidly rising concentration of greenhouse gases in the atmosphere. Density functional theory (DFT) and molecular dynamic simulation investigations are used in this study to examine the adsorption characteristics of SO۲ and NO۲ on zirconia surface. Several global reactivity parameters are analyzed as part of the DFT calculations, including the energy of the highest occupied molecular orbital (EH), the energy of the lowest unoccupied molecular orbital (EL), the separation energy (ΔE), electronegativity (χ), ionization potential (I), electron affinity (A), hardness (η), softness (σ), the global electrophilicity index (ω), the nucleophilicity (ε), the energy of back donation (ΔEb-d) and fraction of electron(s) transfer (ΔNmax). The adsorption/binding energies that come from the interaction between the molecules and the ZrO۲ (۱۱۰) surface are taken into account in the molecular dynamic simulation. Compared to NO۲ (ΔE = ۶.۴۲۴ eV), the zirconia surface is substantially more sensitive to SO۲ (ΔE = ۵.۴۱۵ eV) capture, according to the DFT data. The findings of the quenched molecular dynamic simulations also showed that SO۲ (Eads = -۶۶.۲۳ kcal/mol) is more likely to adsorb on zirconia surface than NO۲ (Eads = -۵۷.۵۰ kcal/mol), despite the fact that both molecules obey the physical adsorption mechanism. S for SO۲ and N for NO۲ respectively bond to the ZrO۲(۱۱۰) surface due to the two molecules' favorable orientation, which is parallel to the surface with angles pointing upward. Zirconium oxide can thus be used as an effective adsorbent for the removal of SO۲ and NO۲ gases from air environments as a result of these discoveries.

کلمات کلیدی:

Greenhouse Gases, Zirconia surface, Molecular Dynamic Simulation, Density functional theory, Physical Adsorption