Styrene Adsorption on Pristine and Modified Smectites: A DFT-D3 Approach for Green Applications

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Effective removal of environmental pollutants remains a critical challenge, particularly for hazardous organic compounds such as styrene. Clay minerals, owing to their high surface area, cation exchange capacity, and versatile adsorption characteristics, have emerged as promising materials for sustainable remediation strategies. Their natural availability, low production cost, and environmentally benign properties further enhance their appeal for practical applications [1]. Among these materials, organoclays have demonstrated remarkable efficiency in capturing both organic and inorganic contaminants, offering robust solutions for pollutant sequestration in water and soil systems [2].

This work examines the adsorption performance of pristine smectite clays, such as montmorillonite (Mnt) and saponite (Sap), in comparison to their functionalized counterparts modified with poly(2-methyl-2-oxazoline) (PMOx) for styrene removal [3]. Using Density Functional Theory (DFT) with the D3 scheme for correction of dispersion forces [4], the adsorption mechanisms, structural stability, and interaction energies for the mentioned hybrid systems based on both pristine and modified smectites were systematically analyzed.

The analysis of the computational results revealed that PMOx-modified smectites (Mnt+PMOx and Sap+PMOx) possess enhanced adsorption affinity and greater structural stability relative to their unmodified counterparts. These results underscore their potential as highly efficient and environmentally sustainable adsorbents. Furthermore, the findings offer important guidance for the rational design of advanced hybrid clay materials aimed at the effective remediation of hazardous organic pollutants.

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