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Insights into the H_2S adsorption on Pt_Y zeolite clusters models

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The properties of zeolites are of significant interest due to their ability to facilitate various chemical processes, particularly in heterogeneous catalysis. Zeolites, with their porous structure and high surface area, can selectively exchange cations within their framework, which allows them to act as efficient catalysts. Zeolites containing metal ions become more active and stable catalysts, making them more useful in industrial processes like refining, petrochemicals, and environmental cleanup. The incorporation of divalent ions can enhance the thermal stability and durability of FAU zeolites, making them highly desirable for industrial catalytic processes. These processes include desulfurizing fuels and purifying biogas by removing H_2S, thereby making biogas a viable renewable fuel source. In this way, the major challenge in the heterogeneous catalysis is catalyst design with good activity, high selectivity, and satisfactory stability [1]. Quantum calculation is effective for studying ion exchange in zeolites due to its ability to provide detailed atomic and electronic insights [2]. The calculations were performed using B3LYP hybrid functional with the basis set Lanl2dz for Pt atom and 6-31+G(d) for Al, H, Si, S and O atoms. The atomic charges were determined based on NBO analysis. The goal of this work is to calculate the geometric parameters, interaction energy and NPA charge for the Pt-FAU_H_2S system. The frequency calculation verified the optimized structure as real minima. In the analysis of the optimized structure, it is observed that H_2S loses a hydrogen atom, which then bonds to an adjacent oxygen atom within the zeolite framework. The calculated interaction energy for the adsorbed H_2S, including the Basis Set Superposition Error (BSSE) correction, is 83.52 kcal/mol. Determining atomic charges is crucial for understanding charge transfer and polarization in adsorption complexes. Analyzing the Natural Population Analysis (NPA) charges revealed a significant electron transfer from the sulfur atom in H_2S to the platinum cation in the zeolite. This indicates a migration of electron density from the adsorbate molecule to the metallic cation, which highlights the strong interaction and potential catalytic activity within the zeolite framework. In conclusion, the analysis demonstrated that H_2S adsorbs onto the zeolite, losing a hydrogen atom that subsequently bonds to an adjacent oxygen atom. The determination of atomic charges proved essential in understanding the charge transfer and polarization effects within the adsorption complex indicating a strong interaction and highlighting the potential catalytic activity of the zeolite framework. This study shows how the structure and electronic properties of a material influence in the adsorption process, offering valuable insights for the design and optimization of zeolite-based catalysts.

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