Adsorption Characteristics of Hydrocarbons (Propylene, n-butane, and Toluene) on Metal cation-exchanged ZSM-5 Zeolites by Computational Analysis

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The adsorption characteristics of vehicle emission adsorbents in hydrocarbon trap (HC trap) was computationally investigated. The adsorbents and adsorbates were cation-exchanged ZSM-5 zeolites and three hydrocarbons (propylene, n-butane, toluene), respectively. Cations such as lanthanum (La), potassium (K), and silver (Ag) were exchanged to provide hydrothermal stability to the zeolite structure. To support the experimentally obtained adsorption characteristics by using TPD (thermal programmed desorption) and TGA (thermogravimetric analysis), a DFT-based molecular modeling was employed. A cluster approximation, where the catalytic active site is cleaved out from the zeolite structure, was employed to save the computational capacity. And the binding enerigies for the physisorption between hydrocarbon species and the cluster were calculated and compared with experimental results.