A first principles study on the catalytic performance of methylcyclohexane dehydrogenation on a monoatomic catalyst

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Abstract	This research explores how methylcyclohexane (MCH) interacts with individual metal atoms M (M= Pt, Pd, and Cu) based on density functional theory (DFT) total energy calculations. We analyzed the adsorption energies of MCH on these metal atoms to understand their stability and reactivity. The results show that MCH prefers to attach to single Pt atoms, which exhibited the strongest adsorption energy. Compared with Pt(111) surfaces, the adsorption energies on Pt atoms were slightly higher, indicating enhanced stability at the nanoscale. Adsorption on Pd and Cu atoms resulted in lower adsorption energies than on Pt. We also focused on the initial step of dehydrogenation, where we studied the removal of one hydrogen atom (H1) from MCH. The presence of a single metal atom significantly lowered the energy required for breaking the C1-H1 bond, with Pt showing the lowest energy barrier compared with Pd and Cu due to the excessive of charge transfer. We analyzed the electronic properties and charge transfer during dehydrogenation, revealing the influence of the metal atom's electronic structure on catalytic behavior. Overall, this research provides valuable insights into how MCH interacts with monoatomic metal catalysts, emphasizing the role of the metal atom's electronic configuration in determining reactivity.
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