Modulation of Fischer-Tropsch Product Selectivity via Various Substrates Supported Rhodium Nanoclusters - A DFT Study

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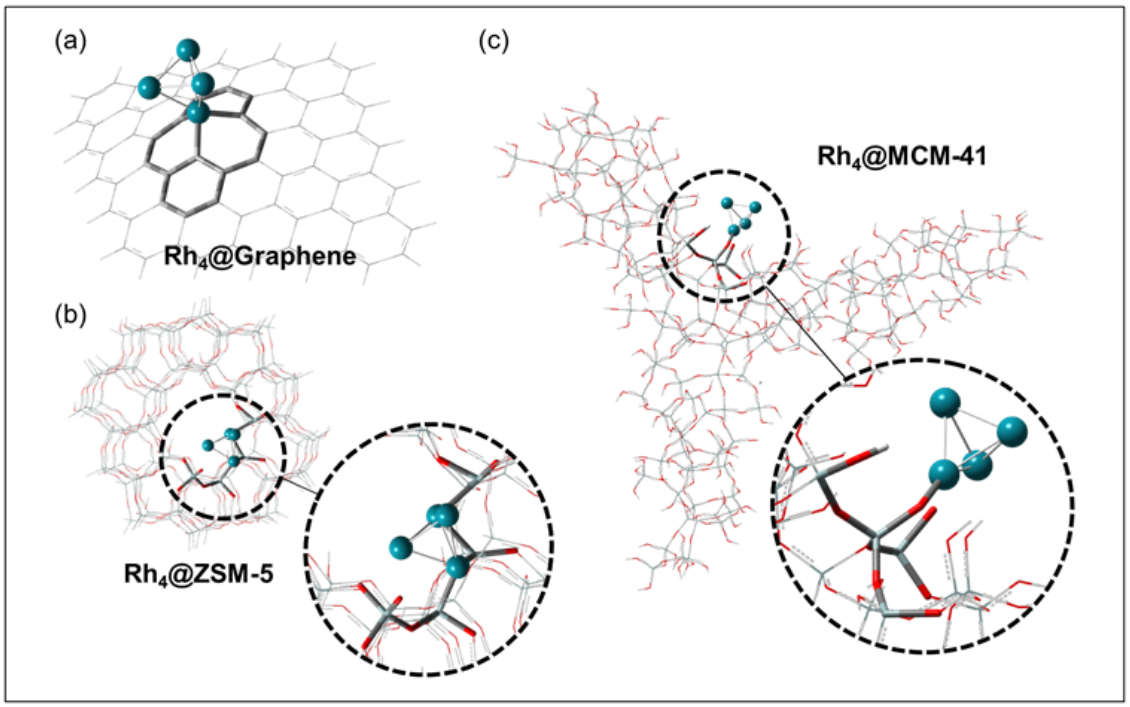
Fischer-Tropsch Synthesis (FTS) converts CO and H_2 into hydrocarbons, offering a viable solution to 21st-century energy challenges. While Rh nanoclusters effectively catalyze FTS, their activity varies significantly depending on support interactions. This study employs density functional theory (DFT) to investigate Rh_4 nanocluster stability on graphene, ZSM-5, and MCM-41. The examination insights the reaction mechanisms of $*CH_x$ formation. We systematically analyze the selectivity of hydrogen-assisted $*CH_xO$ (x = 1, 2, 3) dissociation across these supported systems. It is concluded that the modulation of Rh_4 nanocluster activity through strategic support selection, optimizing energy barriers to develop highly selective FTS catalysts.



References

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