Density functional study of Pt4 clusters adsorbed on a carbon nanotube support

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Abstract: Small clusters on substrates usually exhibit large numbers of configurations separated by relatively small barriers and easily interconvert between such configurations, known as structural fluxionality. We investigate here this property in hybrid catalytic structure: small Pt clusters adsorbed on single-wall carbon nanotube (SWNT) support using density functional calculations. We find that the Pt4 clusters adsorbed on SWNT support exhibit several energetically accessible structural isomers with rather low-energy barriers, resulting in the high degree of structural fluxionality. We find that curvature of SWNT and charge redistribution play important roles in the variation in structure of Pt4 cluster on SWNT. The high degree of structural fluxionality allows the Pt4 clusters on SWNT to interact easily with environmental gas molecules such as CO by adapting their structures. The change in electronic structure via molecular adsorption due to the structural fluxionality and the variation in structure caused by changes in electronic structure are strongly interrelated resulting in the wide variety of dynamic reactions of CO molecules with Pt4 clusters.

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