Sequential Dissociative Chemisorption of H\textsubscript{2} on Ti\textsubscript{13} Cluster\textsuperscript{1}

T.J. DHILIP KUMAR, P. TARAKESHWAR, N. BALAKRISHNAN, Department of Chemistry, University of Nevada Las Vegas, 4505 Maryland Parkway, Las Vegas, NV 89154 USA — Ti nanoparticles have received much attention due to their superior catalytic property in potential hydrogen storage materials for fuel cell applications. In this study, we show that the energetically stable distorted icosahedral Ti\textsubscript{13} cluster has excellent H\textsubscript{2} adsorption and desorption properties and lead to stable structures upon hydrogen cycling. H\textsubscript{2} adsorption initially leads to a highly stable Ti\textsubscript{13}H\textsubscript{20} cluster and on further saturation yields the Ti\textsubscript{13}H\textsubscript{30} cluster. The chemisorbed H atom in Ti\textsubscript{13}H\textsubscript{20} occupies above the face of the triangular planes of Ti\textsubscript{13} whereas in Ti\textsubscript{13}H\textsubscript{30}, H atoms remain dangling above the apex Ti edges. The three coordinated H in Ti\textsubscript{13}H\textsubscript{20} has higher chemisorption and desorption energies than the fully saturated Ti\textsubscript{13}H\textsubscript{30} cluster. This type of multi-center H-bonds with varied chemisorption energies is structurally significant since adsorption and desorption rate processes could be controlled and deserve attention as potential candidates for hydrogen storage materials.

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