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Sequential Dissociative Chemisorption of H_2 on Ti_{13} Cluster[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_{13} cluster has excellent H_2 adsorption and desorption properties and lead to stable structures upon hydrogen cycling. H_2 adsorption initially leads to a highly stable $Ti_{13}H_{20}$ cluster and on further saturation yields the $Ti_{13}H_{30}$ cluster. The chemisorbed H atom in $Ti_{13}H_{20}$ occupies above the face of the triangular planes of Ti_{13} whereas in $Ti_{13}H_{30}$, H atoms remain dangling above the apex Ti edges. The three coordinated H in $Ti_{13}H_{20}$ has higher chemisorption and desorption energies than the fully saturated $Ti_{13}H_{30}$ 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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T.J. Dhilip Kumar
Department of Chemistry, University of Nevada Las Vegas

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