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14. ABSTRACT In this report we provide details on our recent study on enhancing the efficiency of cathode materials for PFME cells. We chose nickel clusters as the prime material because of the following reasons: (1) wide available in the earth crust, (2) cheap, (3) equally active as Pt material, and (4) clusters are very active than bulk. We dope several transition metals (Group VIII B, IB and IIB) in to the Nickel clusters and study their stability and electronic properties, H2 adsorption properties, and H2 dissociation (main process involved at the cathode site). We performed density functional studies of H2 adsorption and dissociation on a series of late transition metal (LTM) doped nickel clusters. The results indicate that the dopant play a major role in modulating the adsorption and dissociation of H2 on the clusters. Results have been submitted, Feb 2011, to the Journal of Physical Chemistry			
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Theoretical studies in enhancing the efficiency of cathode and anode materials in PEMFC (Proton Exchange Membrane Fuel Cells)

In this report we provide details on our recent study on enhancing the efficiency of cathode materials for PEMFC cells. Present day fuel cell use Pt clusters as catalyst. We chose nickel clusters as the prime material because of the following reasons: (1) wide availability in the earth crust, (2) cheap, (3) equally active as Pt material, and (4) clusters are very active than bulk. We dope several transition metals (Group VIIIIB, IB and IIB) in to the Nickel clusters and study their stability and electronic properties, H₂ adsorption properties, and H₂ dissociation (main process involved at the cathode site). We performed density functional studies of H₂ adsorption and dissociation on a series of late transition metal (LTM) doped nickel clusters. The results indicate that the dopant play a major role in modulating the adsorption and dissociation of H₂ on the clusters. Doping late transition metal (LTM) impurity in to nickel clusters results in segregation of dopant due to their higher atomic radius and a charge transfer to occur from the dopant to the nickel center. The NPA analysis (natural population analysis) shows the valence *d* and *p* orbital of the dopant atoms are altered by the donation/back donation of electrons from the nickel center. The binding energy and dissociation energy calculated for the pentamer cluster indicates that their stability are enhanced by doping, while there exists no clear trend for the small cluster due to the quantum size effect.

The chemisorption of H₂ on the clusters occurs at the bridge sites, without any structural and spin change except the Cd doped pentamer. Among the pentamer clusters, Cd, Zn and Au have the lowest chemisorption energy, while Ir and Pt have higher chemisorption energy among the dopant atoms studied. Dopant atoms play a major role in modulating the chemisorption on these clusters. Molecular hydrogen physisorption occurs at the vertex atom with low coordination number which is mainly due to the interaction variation between the *s* orbital of H₂ and the LUMO orbital's of the clusters. The dopant decides the shape of LUMO orbital and the approach of H₂ molecule. Further, a charge transfer was found to occur between the cluster and the H₂ molecule which stabilizes the physisorption.

The computed reaction energies, activation barriers for the dissociation mechanism show dopant such as Rh, Pd, Pt and Au have endothermic reaction energies and low activation barriers, which facilitate the H₂ molecule to undergo a reversible adsorption/dissociation on these metal doped clusters. These results demonstrate that the behavior of chemical dissociation from molecular hydrogen into hydrogen atoms on nickel clusters can be tuned by changing the impurity atoms which can be used to design new nanoscale catalysts with desirable properties.

The work has been submitted to Journal of Physical Chemistry for publication.