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Quantum Chemical Investigation of Hydrogen Isotopes Adsorption on Metal Ion Functionalized Linde Type A and Faujasite Type Zeolites

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Abstract : In the inner fuel cycle system of a nuclear fusion reactor, the Hydrogen Isotopes Removal System (HIRS) plays a pivoted role. It enables the effective extraction of the hydrogen isotopes from the breeder purge gas which helps to maintain the tritium breeding ratio and sustain the fusion reaction. One of the components of HIRS, Cryogenic Molecular Sieve Bed (CMSB) columns with zeolites adsorbents are considered for the physisorption of hydrogen isotopes at 1 bar and 77 K. Even though zeolites have good thermal stability and reduced activation properties making them ideal for use in nuclear reactor applications, their modest capacity for hydrogen isotopes adsorption is a cause of concern. In order to enhance the adsorbent capacity in an informed manner, it is helpful to understand the adsorption phenomena at the quantum electronic structure level. Physicochemical modifications of the adsorbent material enhances the adsorption capacity through the incorporation of active sites. This may be accomplished through the incorporation of suitable metal ions in the zeolite framework. In this work, molecular hydrogen isotopes adsorption on the active sites of functionalized zeolites are investigated in detail using Density Functional Theory (DFT) study. This involves the utilization of hybrid Generalized Gradient Approximation (GGA) with dispersion correction to account for the exchange and correlation functional of DFT. The electronic energies, adsorption enthalpy, adsorption free energy, Highest Occupied Molecular Orbital (HOMO), Lowest Unoccupied Molecular Orbital (LUMO) energies are computed on the stable 8T zeolite clusters as well as the periodic structure functionalized with different active sites. The characteristics of the dihydrogen bond with the active metal sites and the isotopic effects are also studied in detail. Validation studies with DFT will also be presented for adsorption of hydrogen on metal ion functionalized zeolites. The ab-inito screening analysis gave insights regarding the mechanism of hydrogen interaction with the zeolites under study and also the effect of the metal ion on adsorption. This detailed study provides guidelines for selection of the appropriate metal ions that may be incorporated in the zeolites framework for effective adsorption of hydrogen isotopes in the HIRS.

Keywords : adsorption enthalpy, functionalized zeolites, hydrogen isotopes, nuclear fusion, physisorption
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