World Academy of Science, Engineering and Technology
International Journal of Materials and Metallurgical Engineering
Vol:18, No:03, 2024

Efficient Hydrogen Separation through Pd-Pt Membrane

Authors : Lawan Muhammad Adam, Abduljabar Hilal Alsayoud

Abstract : One of the most promising techniques to produce pure hydrogen is through a palladium-based membrane (Pd-membrane). Density functional theory (DFT) is employed in this work to examine how the physical and chemical adsorption properties of hydrogen on the surface of Pd-Pt can be mutated in the presence of contaminating gases, CH_4, CO, and CO_2. The main target is to survey the energy topology related to hydrogen adsorption while adjusting the stages of freedom in both the structure and composition. The adsorption sites, crystal plane of the slab, and relative orientation of the adsorbed molecules on its surface, as well as various arrangements of adsorbed species, have been considered in this study. The dependency of hydrogen adsorption on surface coverage is studied. The study demonstrated the physical adsorption energies of the molecules on the surface concerning the different coverages of hydrogen atoms. The most stable combinations of the adsorption sites (Top, Hollow, and Bridge) with various orientations of gaseous molecules on the Pd-Pt surface were identified according to their calculated energies. When the binding of contaminating gaseous species to the Pd-Pt surface and their impact on the physical adsorption energies of the H_2 are examined, it is observed that the most poisonous gas relative to all other gases modifies the energetics of the adsorption process of hydrogen on the surface.

Keywords : DFT, Pd-Pt-membrane, H_2, CO, CO_2
Conference Title : ICMSE 2024 : International Conference on Materials Science and Engineering
Conference Location : Tokyo, Japan
Conference Dates : March 18-19, 2024