Abstract

Through first-principles modeling, we have investigated both the Hydrogen (H) adsorption and incorporation into clean Zr(0001), as well as the effect of the monovacancy and the impurities impact on the hydrogen diffusion into Zr(0001). The achieved results confirm that HCP and FCC sites are energetically the most stable for H adsorption E_{ads}(H), while the most probable H incorporation sites are Octahedral and Tetrahedral sites (inOcta and inTetra). The monovacancy reduces the E_{ads}(H) at the FCC site. At $\Theta = 0.25$ monolayer (ML), the additional Fe, Ni, and Nb-doped Zr (0001) increased the incorporation energy E_{incorp}(H) at inTetra site, while Sn and Si reduced it. Cr and Nb remarkably decrease the Minimum Energy Path (MEP) energy of H migration. The obtained results are intrinsic and advantageous for hydrogen storage in alloys based Zr, while these impurities could harm the cladding material by facilitating hydrides formation