Poster Session | A. Advances in Materials Theory for Multiscale Modeling

[PO-A1]Poster Session 1

Symposium A

2018年10月29日(月) 17:45 ～ 20:00 Poster Hall

[P1-06]First-principles investigation of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface

○Zhong-min Wang, Yang Wu, Qingrong Yao, Yan Zhong, Chaohao Hu, Huaiying Zhou (Guilin University of Electronic Technology, China)

Based on sequential study of the surface model, surface-model slab, H-adsorption sites, and H-diffusion coefficient (D), we investigate the most likely process of atomic hydrogen adsorption and diffusion on/into Mo-doped Nb (100) surface/subsurface (in the $Nb_{12}Mo_4$ case) via first-principles. Our results reveal that the (100) surface is the most stable Mo-doped Nb surface with the smallest surface energy (2.75 J/m^2). Hole sites (HSs) in the Mo-doped Nb (100) surface are H-adsorption-favorable mainly due to their large adsorption energy (4.27 eV), and the H-diffusion path should preferentially be HS→TIS (tetrahedral interstitial site) over HS→OIS (octahedral interstitial site) because of the correspondingly lower H-diffusion energy barrier. With respect to a pure Nb (100) surface, the Mo-doped Nb (100) surface has a smaller energy barrier along the HS→TIS pathway (0.31 eV) and larger H-diffusion coefficient (5.65×10^{-10} m^2s^{-1}).