Abstract:

Molecular and atomic oxygen diffusion on uranium mononitride UN(001) surface was studied. The more favorable bridge site corresponding to the oxygen diffusion on UN(001) clean surface was then checked under several surface states such as UN(001) surfaces including uranium or nitrogen vacancies. First principle calculation based on density functional theory (DFT) was used with the generalized gradient approximation (GGA) to describe the exchangecorrelation and the projector-augmented wave (PAW) as pseudo potential. Molecular and atomic potential energy surfaces (PES) corresponding to the interaction between respective molecular (O2) or atomic oxygen (O) and UN(001) surface states at several positions of the surface were used to study and identify the more favorable adsorption sites. The dissociation of molecular oxygen approaching UN(001) surfaces both clean or defected was proved for different orientation of the molecule with both atoms adsorbed on the surfaces. The more ability of oxygen adsorption on UN(001) nitrogen vacancy surface compared to other UN(001) surfaces states was confirmed. Considering more N vacancies on UN(001) surface and more O atoms diffusion, our results show that adsorption energies per O atom decrease with the rise in N vacancies and increase with increasing O atoms diffusion