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

[P1-01]The Coadsorption Effect of Cl- and H_2O on the Various Defect Al_2O_3 Film Surface

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First-principles calculations have been performed on the perfect surface, point-defect surface, step-defect surface, layer-defect surface of Al_2O_3 film with water molecules and chloride ions. The coadsorption mechanism has effect on the reaction and erosion of the surface. The adsorption energies (E_{ads}), stable adsorbed sites, binding of film, charge transfer, reactants and products, activation energies and transition states are calculated and discussed. The results evidence that for the perfect Al_2O_3 surface, the critical monolayer of Cl- is 3/7, the E_{ads} decrease in three steps, each E_{ads} step only relate to the adsorbed site and the morphology. For point-defect surface, substitution point defects are more sensitive than vacancy point defects for reaction and erosion. The species of products depend on the energy barrier and orientation of water. For step-defect surface, Al1 step-defect and Al3 step-defect surfaces prefer to obtain Al-H_2O compounds, while O2 step-defect surface prefers to form Al-Cl products. There is no obvious linear relationship between the number of products and the number of steps. For layer-defect surface, when low concentrations of Cl ions reach the surface, they prefer to erode the Al layer-defect surface with producing Al-Cl compounds, while they prefer to interact with H_2O upon the O layer-defect surface.