7th African Conference on Non Destructive Testing (ACNDT) & the 5th International Conference on NDT and Materials Industry and Alloys (IC-WNDT-MI)

2016

DFT study of F atom adsorption on Si(001) surface

Lemya. Bouamama, Amel. Lounis, Abdelhamid. Ziane, Arezki. Mokrani

Abstract : We have investigated the initial adsorption of an fluorine (F) atom on Si(001) surface by means of first-principles calculations using pseudopotential method implemented in SIESTA code. Three high-symmetric adsorption sites of F on Si(100) were examined : top, bridge and hollow sites. For an F atom adsorbed on perfect Si(001) surface, we found that F atom prefer the bridge adsorption site with a high adsorption energy of 6.47eV. However, in the relaxed case, the adsorption of an F atom leads to a Si(001)-2×1 surface reconstruction and the most stable adsorption site corresponds to the dangling bond site of a Si(100) surface top layer. The Si-F bond is calculated to be 1.67 Å and the adsorption energy of the F atom is evaluated to be 6.51eV.

Keywords : DFT, SIESTA, Silicon, fluorine, adsorption