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The adsorption of halogen molecules on Ti (110) surface

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Abstract

Adsorption of halogen on the metal surface has received much attention due to its technological applications and major relevance for material surface processing, corrosion protection and etching. In this work, first-principle approach was used to investigate the interaction of halogen molecules on Ti (110) surface. The present results revealed that adsorption of the halogen molecule is exothermic and occurs by dissociation bonding. The HF molecule was found to be more thermodynamically stable than the HI molecule. In addition, our results revealed that the adsorption of halogen ions on Ti (110) surface is energetically favourable than the adsorption of halogen molecule. The possible adsorption sites were tested, and the top site position was found to be the most favourable followed by the hollow and bridging site for both halogens. Furthermore, the results showed the linear relationship between adsorption energy strength and charge transfer. Also, the density of states and charge density difference was studied to investigate the electronic interaction. The charge redistribution showed an electron depletion on Ti atom and charge accumulation on the halogen region.