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Computer simulation study of HF molecule adsorption on TiO2 rutile surfaces

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Hydrofluoric acid is a candidate that can be used for etching metal oxide surface due to its strong corrosive qualities, However, etching phenomenon is not well understood at the atomistic level. Investigation of HF interaction with TiO2 rutile lower surface index is important for enhancing the etching mechanism. Adsorption geometries and energies of HF on TiO2 rutile lower surface index have therefore been investigated using density functional theory employing CASTEP code. It was found that HF chemically adsorbed on TiO2 surfaces to form Ti-F bond and hydroxyl molecule. The surface (110) was found to be more active in HF adsorption with lower adsorption energy and large charge transfer. In addition, all these surfaces found to have higher adsorption ability with the increasing number of HF molecules. Charge analysis indicated that the dissociated of F atom attract electrons and induced the work function due to the higher electronegativity of fluorine atom. This gives evidence that the adsorption of HF molecules on TiO2 surfaces is by chemisorption.

Apply to be
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yes

Level for award
 (Hons, MSc,
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PhD

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