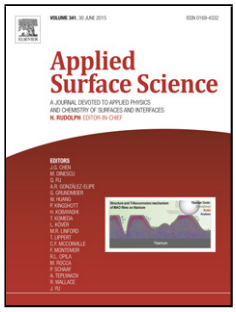

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The role of the defect on the adsorption and dissociation of water on graphitic carbon nitride

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Abstract

Graphitic carbon nitride (g-C_3N_4) as a potential photocatalyst for the water splitting has the focus of numerous experimental and theoretical studies. In the process of water splitting, water/C_3N_4 interface plays the key role in the process, while the detailed mechanism, such as how water adsorbs and dissociates on the metal-free C_3N_4, is still unclear. Here how water interacts with the defect g-C_3N_4 was studied employed both density functional theory (DFT) and molecular dynamics calculations which show that water monomer, dimer, and clusters with three and four molecules at the defect site can form a stable coplanar structure with the g-C_3N_4 sheet. The clusters help to stabilize the adsorption at the defect site. Molecular dynamics simulations show that on the perfect g-C_3N_4 sheet water does not dissociate but on the defect g-C_3N_4 sheet do. There are two reoriented water layers near the g-C_3N_4 sheet because of the interaction between water and the g-C_3N_4 sheet. Our findings indicate that the defect within g-C_3N_4 plays a key role in the adsorption and dissociation of water.

1. Introduction

Solar energy, as a renewable and environment-friendly energy, has been widely thought as the