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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-C₃N₄) as a potential photocatalyst for the water splitting has the focus of numerous experimental and theoretical studies. In the process of water splitting, water/C₃N₄ interface plays the key role in the process, while the detailed mechanism, such as how water adsorbs and dissociates on the metal-free C₃N₄, is still unclear. Here how water interacts with the defect g-C₃N₄ 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-C₃N₄ sheet. The clusters help to stabilize the adsorption at the defect site. Molecular dynamics simulations show that on the perfect g-C₃N₄ sheet water does not dissociate but on the defect g-C₃N₄ sheet do. There are two reoriented water layers near the g-C₃N₄ sheet because of the interaction between water and the g-C₃N₄ sheet. Our findings indicate that the defect within g-C₃N₄ 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

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