DFT Studies of the Photocatalytic Properties of MoS_2-Doped Boron Nitride Nanotubes for Hydrogen Production

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Abstract

This study investigated the photocatalytic properties of MoS_2-doped boron nitride nanotubes (BNNTs) for overall water splitting using popular density functional theory (DFT). Calculations of the structural, mechanical, electronic, and optical properties of the investigated systems were performed using both the generalized gradient approximation and the GW quasi-particle correction methods. In our calculations, it was observed that only (10, 10) and (12, 12) single-walled BNNTs (SWBNNTs) turned out to be stable toward MoS_2 doping. Electronic property calculations revealed metallic behavior of (10, 10)-MoS_2-doped SWBNNTs, while the band gap of (12, 12) SWBNNT was narrowed to 2.5 eV after MoS_2 doping, which is within the obtained band gaps for other photocatalysts. Hence, MoS_2 influences the conduction band of pure BNNT and improves its photocatalytic properties. The water-splitting photocatalytic behavior is found in (12, 12) MoS_2-doped SWBNNT, which showed higher water oxidation (OH^-/O_2) and reduction (H^+/H_2) potentials. In addition, optical spectral calculations showed that MoS_2-doped SWBNNT had an optical absorption edge of 2.6 eV and a higher absorption in the visible region. All of the studied properties confirmed MoS_2-doped SWBNNT as a better candidate for next-generation photocatalysts for hydrogen evolution through the overall water-splitting process.