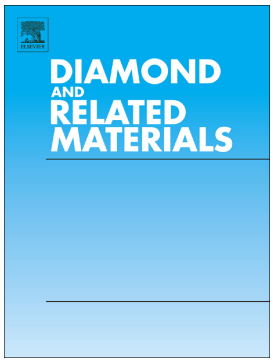

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Potential application of a porous graphitic carbon nitride as an organic metal-free photocatalyst for water splitting

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Highlights

• The electronic structures and optical properties of C_2N-*h*2D, and the possibility of C_2N-*h*2D as an active photocatalyst for hydrogen generation through water splitting.

• In order to absorb more visible light, we further analyzed a series of methods, such as applying tensile, multilayer stacking and doping with boron, oxygen, phosphorus and sulfur.

• The band arrangements and optical absorption properties of the doped materials reveal that the boron and oxygen doped C_2N-*h*2D can effectively extend the range of light absorption, and therefor enhance the photocatalytic efficiency.

Abstract

The new carbon nitride material (C_2N-*h*2D) has been synthesized experimentally by Mahmood et al (Nature Communications, 2015, 6, 6486), however, there is still no study regarding its application as a photocatalyst for water splitting. Herein, we studied the electronic structures and optical properties of C_2N-*h*2D, and explored the possibility of C_2N-*h*2D as an active photocatalyst for hydrogen generation through water splitting. On the basis of our calculation results, the C_2N-*h*2D is suggested to be a direct band gap semiconductor. The positions of the CBM and the VBM are ideal with respect to the standard water redox potentials. More importantly, C_2N-*h*2D can effectively absorb visible light, indicating a promising photocatalyst for water splitting. In order to absorb more visible light, we further analyzed a series of methods,