Harnessing DFT Technologies for Rapid Screening and Design of Efficient Carbon Nitride-Based Photocatalysts

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The growing demand for finding alternative and renewable resources of energy has sparked interest in speeding up the catalyst selection for the Hydrogen Evolution Reaction (HER). Density Functional Theory (DFT) is a computational physics and chemistry tool that helps in determining the chemical and electronic properties of the material while saving time, money, and effort. Herein, C3N5 was investigated as an efficient photocatalyst for the HER by identifying the active sites and calculating the band gap, light absorption, and Gibbs free energy. DFT is used through the Vienna ab initio Simulation Package (VASP), facilitating the Generalized Gradient Approximation (GGA) functional through the Linux interface Shaheen workstations at a high performance supercomputer facility. The most active site of was found to be -0.06 eV, surpassing the benchmark photocatalyst platinum. By identifying the active sites, doping the material using Single Atom Adsorption was facilitated. When C3N5 was doped with Ni, the Gibbs free energy enhanced to -0.03 eV and the band gap reduced to 1.93 eV, outperforming platinum and bare C3N5. Through the data gained from DFT calculations, the DFT-based Machine Learning (ML) for catalysis program (DMCP), was trained to identify the most suitable single atom catalyst that should be tested. This hybrid DFT-ML approach represents a paradigm shift in catalyst development, empowering scientists to tackle complex challenges in energy conversion, environmental remediation, and industrial processes with unparalleled efficiency and speed without compromising accuracy and quality.

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