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First–Principles Study of Semiconductor-Based Photocatalyst Materials for Environmental Remediation

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Due to increasingly global environmental and energy crises, visible light semiconductor photocatalyst with a tunable bandgap and optical properties have received attention. For this reason, developing efficient and cost–effective photocatalysts for environmental remediation is a growing need, and semiconductor photocatalysts have now received more interest due to their excellent photocatalytic stability and activity. The charge transfer, catalytic stability, electronic and optical properties of several semiconductor–based photocatalyst materials were systematically studied using first–principles study. All the calculations were performed using the Cambridge Serial Total Energy Package (CASTEP) code [1] implemented in Materials Studio 2016 [2] with the plane–wave ultrasoft pseudopotentials method [3] and Perdew–Burke–Ernzerhof (PBE) functional for the exchange and correlation contribution [4]. All the simulations were done using the resources provided by the Centre for High Performance Computing (CHPC), Rosebank, Cape Town [5]. The proposed photocatalyst materials show high photocatalytic activity under visible light irradiation with good stability and reduced bandgap compared to the bulk semiconductor. The heterostructures formed a type–II band alignment to accelerate the interfacial charge transfer process and the photocatalytic activity. By comparing the relative ratio of effective mass and band alignment results, we could conclude that heterostructures have not only superior mobility of charge carriers, but also higher separation of photoinduced electrons and holes.

References
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