Type II van der Waals Heterostructures of SiC/Al_2OS monolayers for Photocatalysis and Optoelectronics Applications

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Background

- Global energy demands and consumption have increased over the past few years due to a significant increase in industrialization, urbanization and population.[1]
- The creation of photocatalytic hydrogen through water splitting under light irradiation is receiving great attention as an alternative energy to replace fossil fuels.[2]
- Silicon carbide (SiC) has emerged as a photocatalyst material for effective H_2 evolution due to its electronic, structural, mechanical and optical properties.[1]
- 2D Janus Al_2OS monolayer has been theoretically proved that a strong visible light absorption, desirable bandgap that can help improve hydrogen evolution reaction.[3]

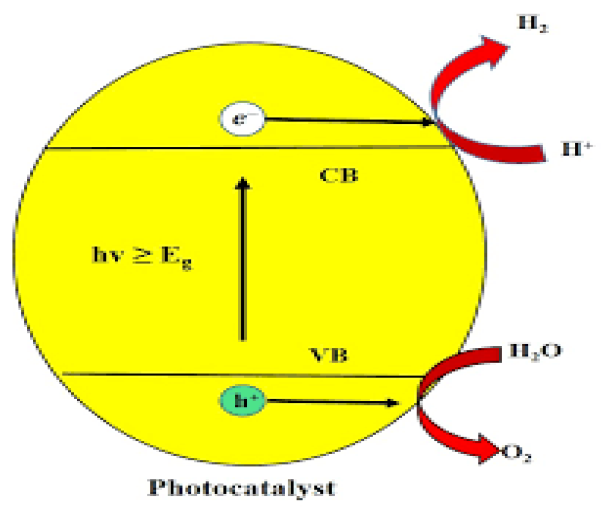

Figure 1 : Mechanism of photocatalytic water splitting.

Aim and Objectives

Aim

- To investigate the electronic properties of van der Waals heterostructure of SiC and Al_2OS monolayers for photocatalytic and optoelectronic applications.

Objectives

- To evaluate the photocatalytic potential by comparing the band edges with redox potential of water.
- To enhance the charge separation and transfer capabilities of photocatalytic materials.

Computational Details

- Solving the kohn sham equation in DFT with plane wave basis set. The Quantum ESPRESSO code was used to perform DFT calculations. Vacuum thickness 30 Å
- The **cut off energy** was set as **45 Ry** and the Monkhorst–Pack **k point mesh** of **6 × 6 × 1** and **15 × 15 × 1** was used for all the optimization processes and electronic properties calculations, respectively. Heyd–Scuseria–Ernzerhof (HSE06) hybrid functional was used to accurately predict the optical and electronic properties.
- norm conserving Vanderbilt pseudopotentials to account for the electron–ion interaction
- The interlayer vdW interactions and dipole were treated using the dispersion corrections of Grimme DFT - D3 method.

Results and Discussion

Structure Geometry

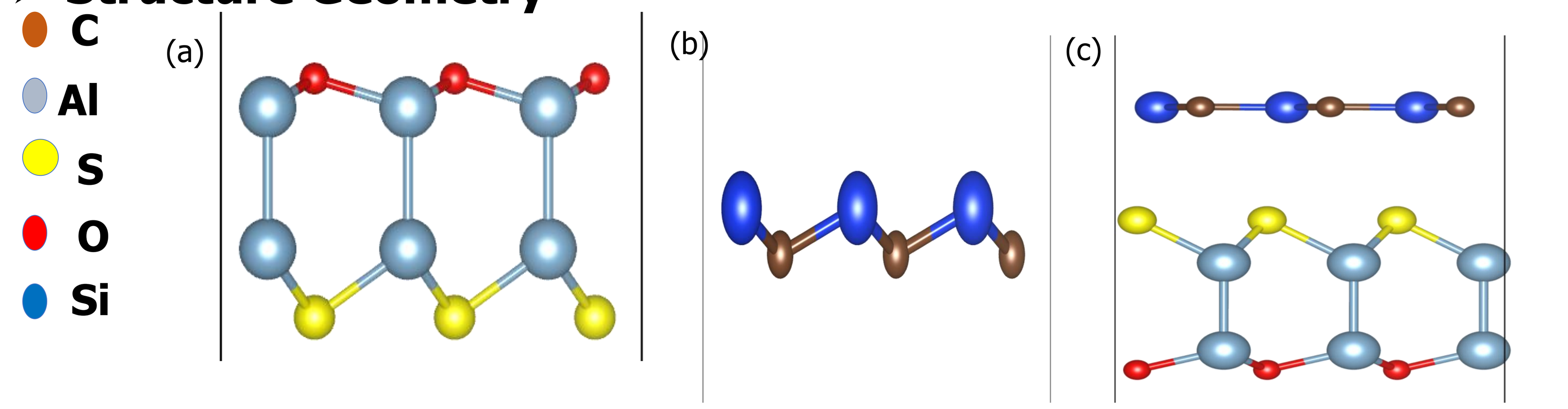

Figure 2 : Optimized side view of (a) Al_2OS monolayer (b) SiC monolayer and (c) The side and top view of SiC/Al_2OS heterostructure

Table 1: Lattice parameters ($a=b$) of SiC and Al_2OS monolayers and SiC/Al_2OS heterostructure.

	(a=b) (Å)	Experimental (Å)	Lattice mismatch (%)
Al_2OS	3.22	3.28	-
SiC	3.07	3.11	-
SiC/Al_2OS	3.17	-	2.39

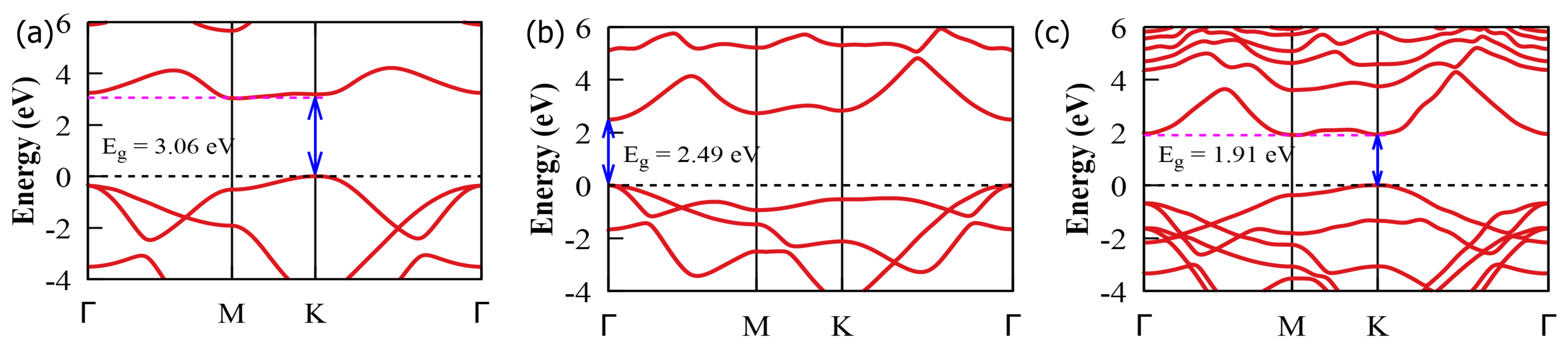

Figure 3 : The calculated band structure of (a) SiC (b) Al_2OS and (c) SiC/Al_2OS heterostructure

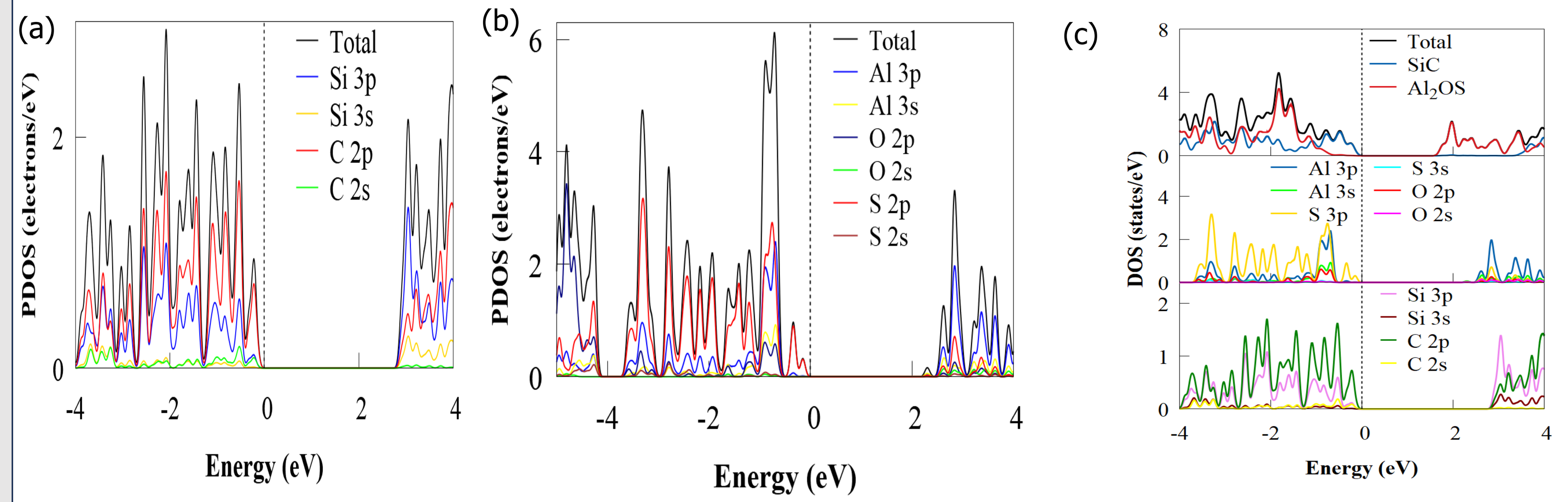

Figure 4 : The calculated projected density of state of (a) SiC (b) Al_2OS and (c) SiC/Al_2OS heterostructure

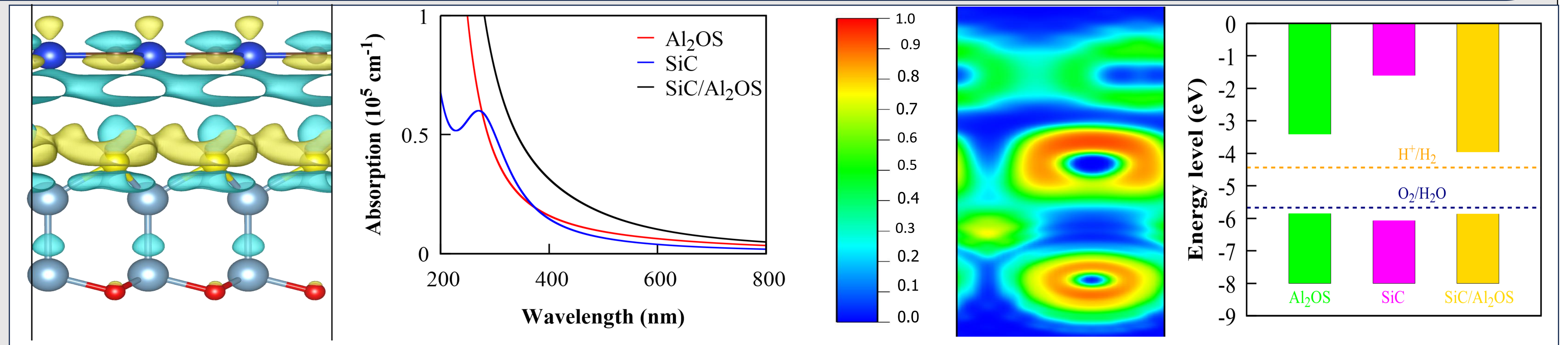

Figure 5: (a) The charge density difference of SiC/Al_2OS heterostructure with the blue and yellow being charge accumulation and depletion, respectively (b) The calculated light absorption spectra of SiC/Al_2OS heterostructure and the monolayers. (c) Electron localization function of SiC/Al_2OS heterostructure and (d) band alignment for the SiC/Al_2OS heterostructure

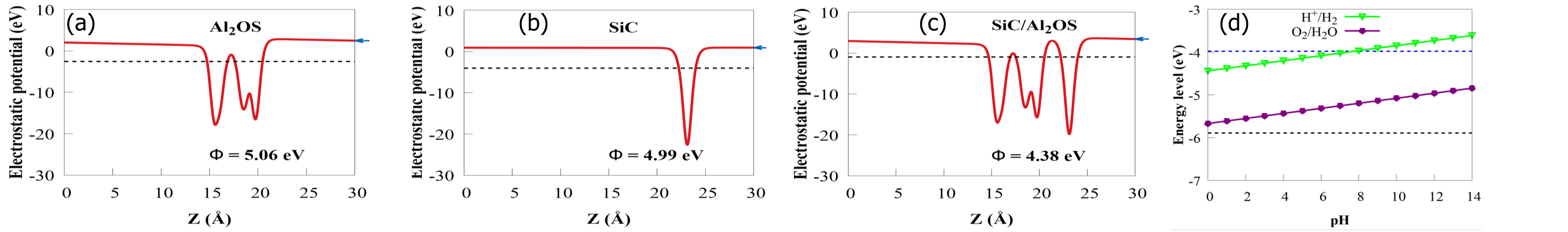

Figure 6: Work function of (a) SiC monolayer (b) Al_2OS monolayer (c) SiC/Al_2OS heterostructure. (d) Band edge potentials against a normal hydrogen electrode at pH = 0 of SiC/Al_2OS vdWHs.

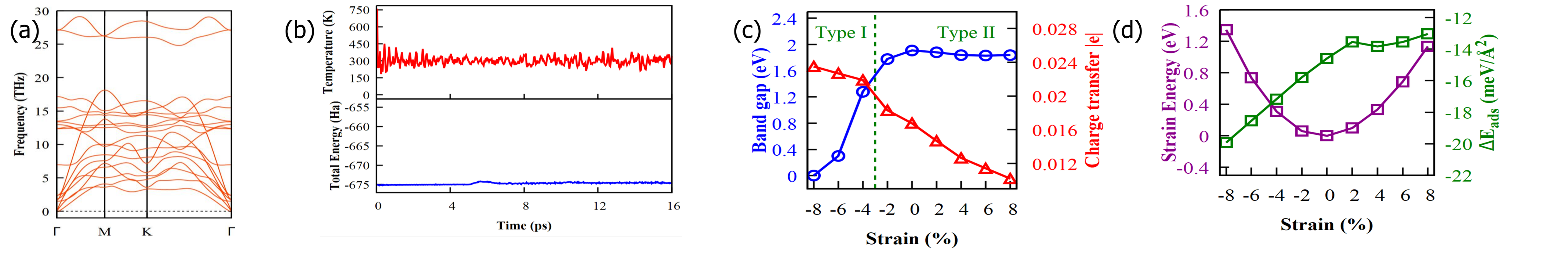

Figure 7 : Snapshots of (a) Phonon dispersion of SiC/Al_2OS vdWHs (b) molecular dynamics at 300K (c) Variation of the interfacial binding energy and the strain energy, and (d) changes in the charge transfer and the band gap energy

Conclusion

- SiC/Al_2OS heterostructure exhibits a direct bandgap of 1.91 eV with a type-II band alignment, which can effectively separate and transfer charge carriers, thereby enhancing the photocatalytic activity.

1. Opoku, F., Akoto, O., Kwaansa-Ansah, E. E., Asare-Donkor, N. K., & Adimado, A. A. (2023). Rational design of 2D/2D CS/SiC van der Waals type-II heterojunctions: a visible-light-driven photocatalyst for hydrogen production. Materials Advances, 4(8), 1949-1963.
2. Ng, K. H., Lai, S. Y., Cheng, C. K., Cheng, Y. W., & Chong, C. C. (2021). Photocatalytic water splitting for solving energy crisis: Myth, Fact or Busted?. Chemical Engineering Journal, 417, 128847.
3. Opoku, F., Aniagyei, A., Akoto, O., Kwaansa-Ansah, E. E., Asare-Donkor, N. K., & Adimado, A. A. (2023). Investigation of 2D Janus Al_2OS/Ga_2SSe van der Waals heterojunction as next-generation thermoelectric and photocatalytic devices. Next Materials, 1(4), 100042.