

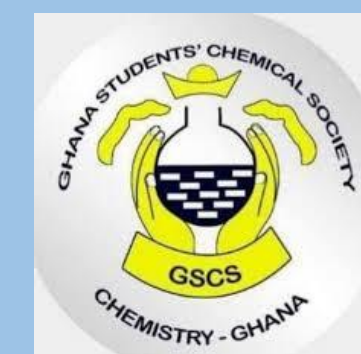


Electronic and Photocatalytic Properties of a two-dimensional BP/MoSSe van der Waals Heterostructure: A First-Principles Study

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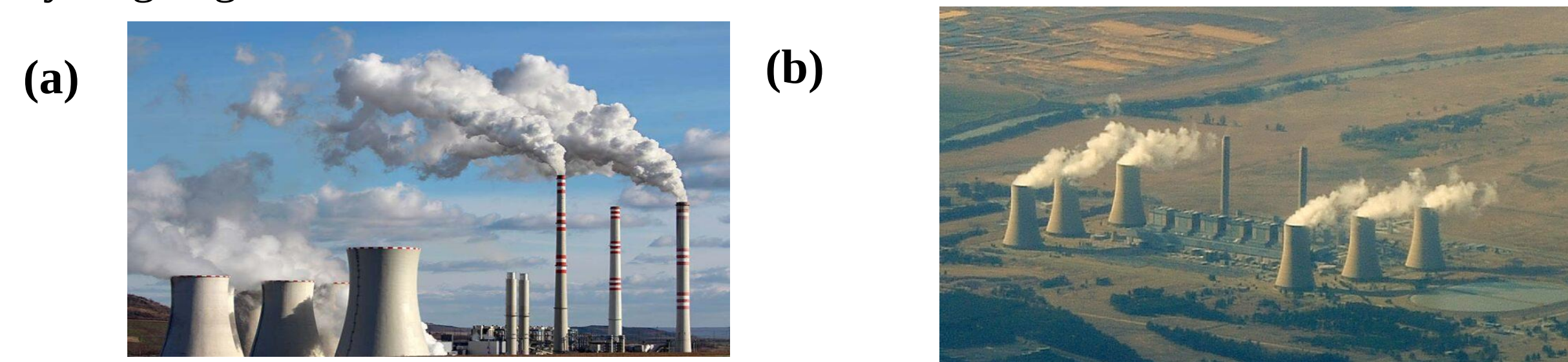
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Introduction

- ❑ The global dependence on the use of exhaustible fossil fuel has made the search for renewable and sustainable energy more urgent.^[1]
- ❑ The combustion of fossil fuels typically results in substantial CO₂ emissions, which contribute to environmental issues such as the greenhouse effect.^[2]
- ❑ Photocatalytic water splitting into H₂ has emerged as a clean and promising energy source to address global environmental pollution.^[3]
- ❑ This has led to the exploration of two-dimensional (2D) materials capable of photocatalytically evolving hydrogen gas from water.



Figures 1 (a,b) Combustion of fossil fuel.

Aim

- ❑ The aim of this work are to study the formation of a heterostructure involving MoSSe and BP, focusing on characterizing the electronic properties and assessing it photocatalytic activity in H₂ evolution reactions.

Objectives

- ❑ To optimize the BP/MoSSe heterostructure.
- ❑ To investigate the electronic and optical properties of BP/MoSSe heterostructure.
- ❑ To explore the photocatalytic performance of the BP/MoSSe heterostructure in the evolution of H₂ from water.

Computational tools



Results and Discussion

Geometry And Structural Stability

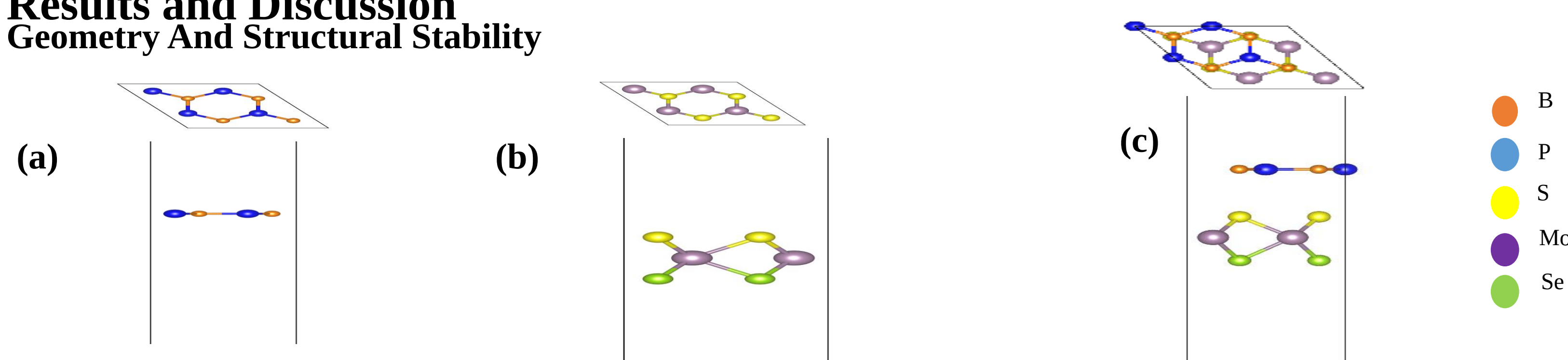


Figure 2. The optimized side view structure of (a) BP sheet (b) MoSSe sheet and (c) BP/MoSSe heterostructure. The brown, blue, green, yellow, and violet are B, P, Se, S, and Mo respectively.

Table 1. The calculated lattice parameters of BP, MoSSe and BP/MoSSe heterostructures

	(a=b) Å	Experiment (Å)
BP	3.26	3.21
MoSSe	3.18	3.25
BP/MoSSe	3.22	-

Electronic structures

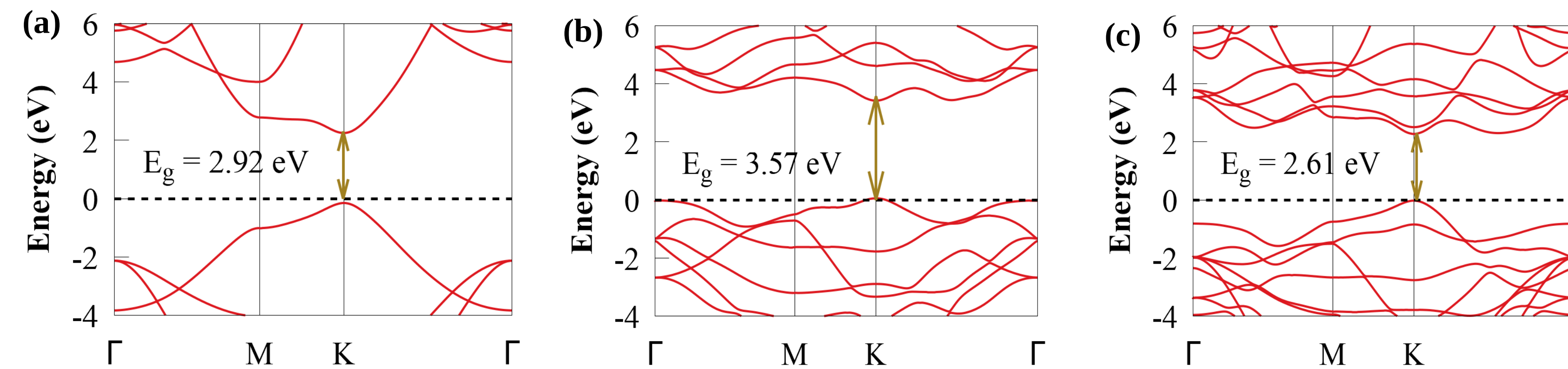


Figure 3. The calculated HSE06 band structure of (a) BP, (b) MoSSe and (c) BP/MoSSe heterostructure

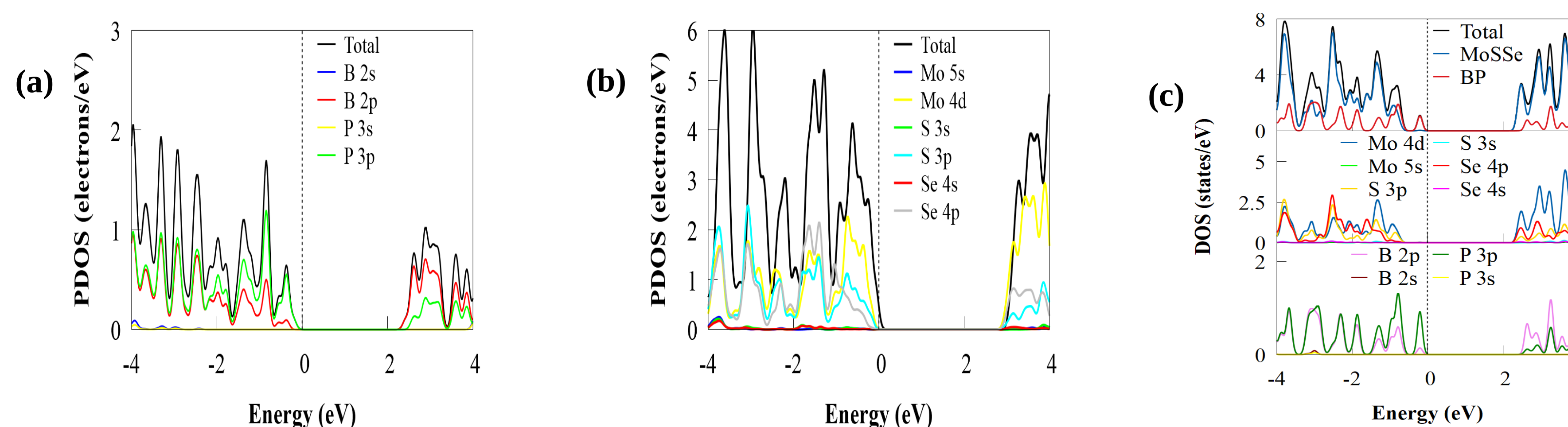


Figure 4. The calculated density of state of (a) BP, (b) MoSSe and (c) BP/MoSSe heterostructure

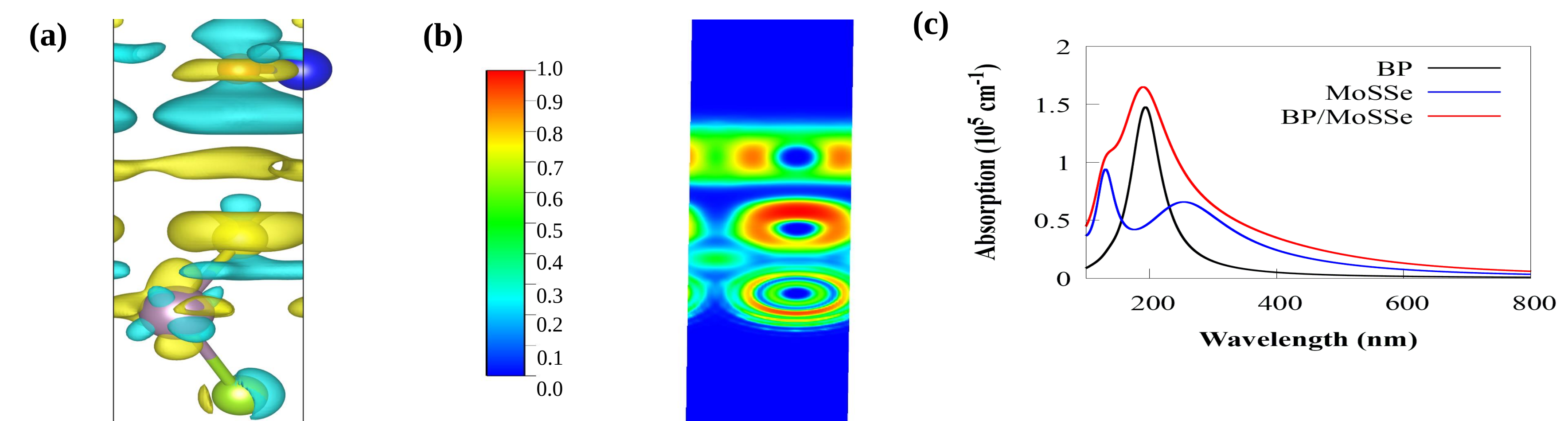


Figure 5. (a) The charge density difference of BP/MoSSe heterostructure. The yellow and the blue region depicts charge accumulation and charge depletion, respectively. (b) The electron localization function of BP/MoSSe heterostructure. (c) The calculated optical absorption spectrum of BP, MoSSe, and BP/MoSSe.

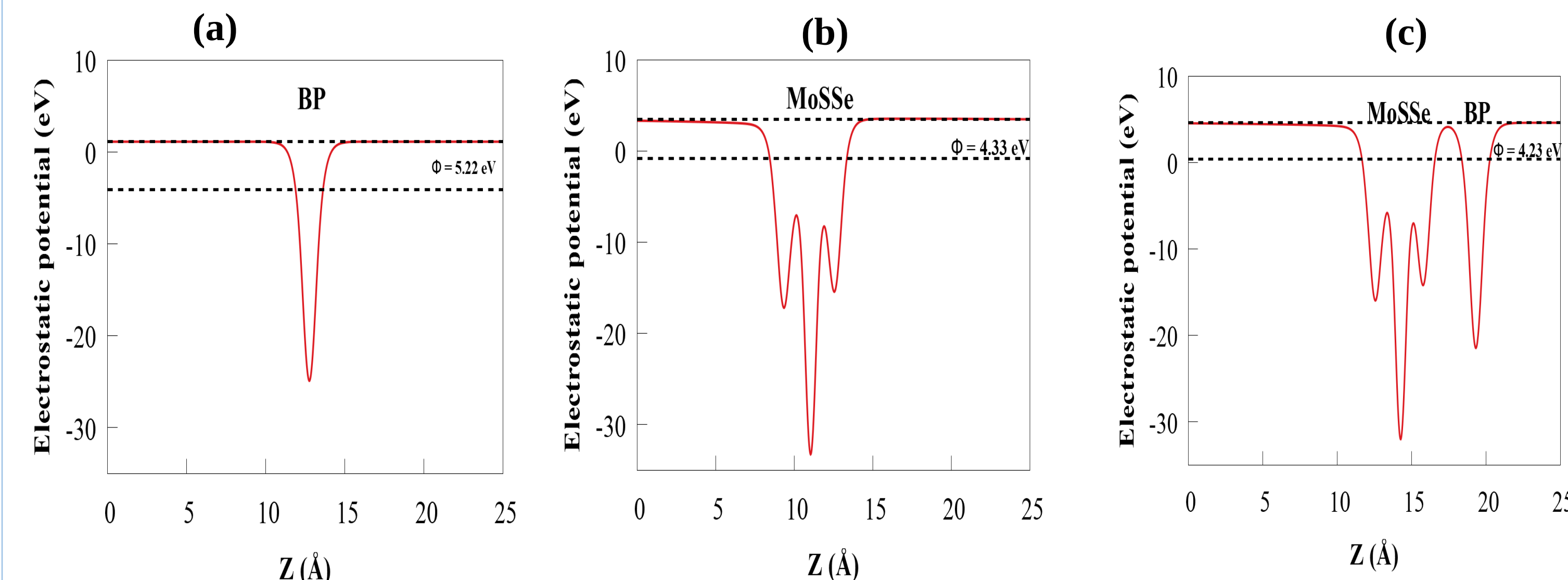


Figure 6. The calculated work function along the Z-direction of (a) BP, (b) MoSSe and (c) BP/MoSSe heterostructure.

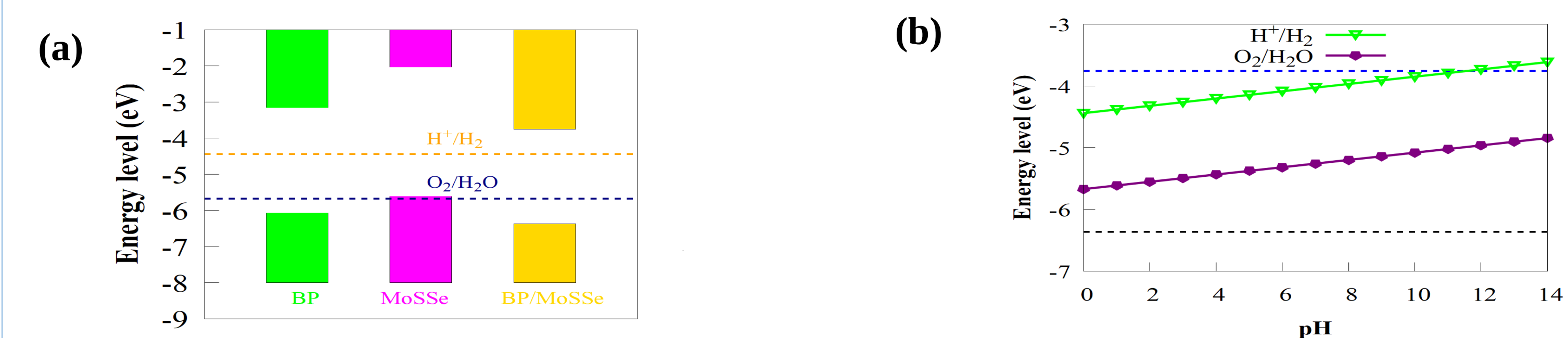


Figure 7. (a) Band alignments of BP, MoSSe, and BP/MoSSe vdW heterostructure. (b) Band alignments of BP/MoSSe vdW heterostructure against pH.

Conclusion

- ❑ Theoretically, BP was used to modify MoSSe by decreasing carrier charge recombination, bandgap, and increasing light absorption.
- ❑ The improved electronic, optical, and photocatalytic properties of BP/MoSSe heterostructure make it possible to be used in water splitting applications and efficient electronic devices.

References

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Acknowledgement



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