Tuning the properties of Janus van der Waals hetero structures by varying interface Terminations

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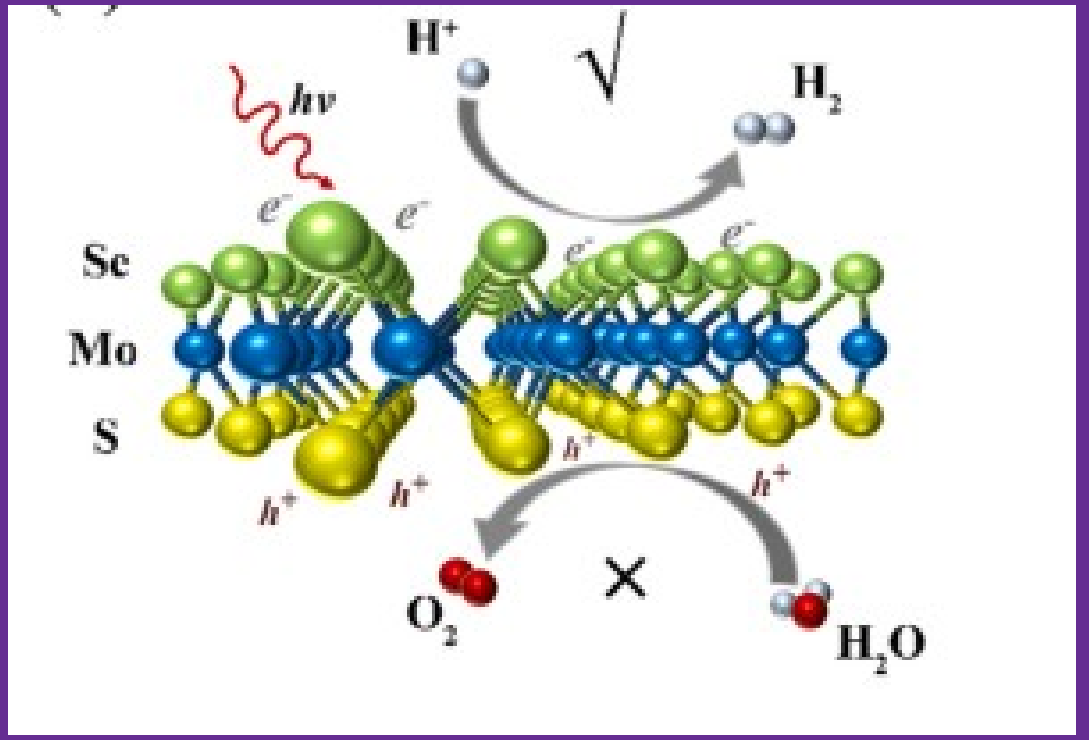
2D Janus Semiconductors and photocatalysis



A.-Y. Lu, et al., Nature Nanotech.12, 744 (2017)

Advantages

1. Indirect to direct band gap transition

2. The out-of-plane broken symmetry and the permanent induced vertical dipole can drive distinct unique quantum phenomena

3.Excellent candidates for heterogeneous photocatalysis owing to the possibility of tuning the morphology

4. Excellent optoelectronic properties due to the chemical characteristics, quantum confinement and the dominant spin-orbit coupling at lower thicknesses

Challenges

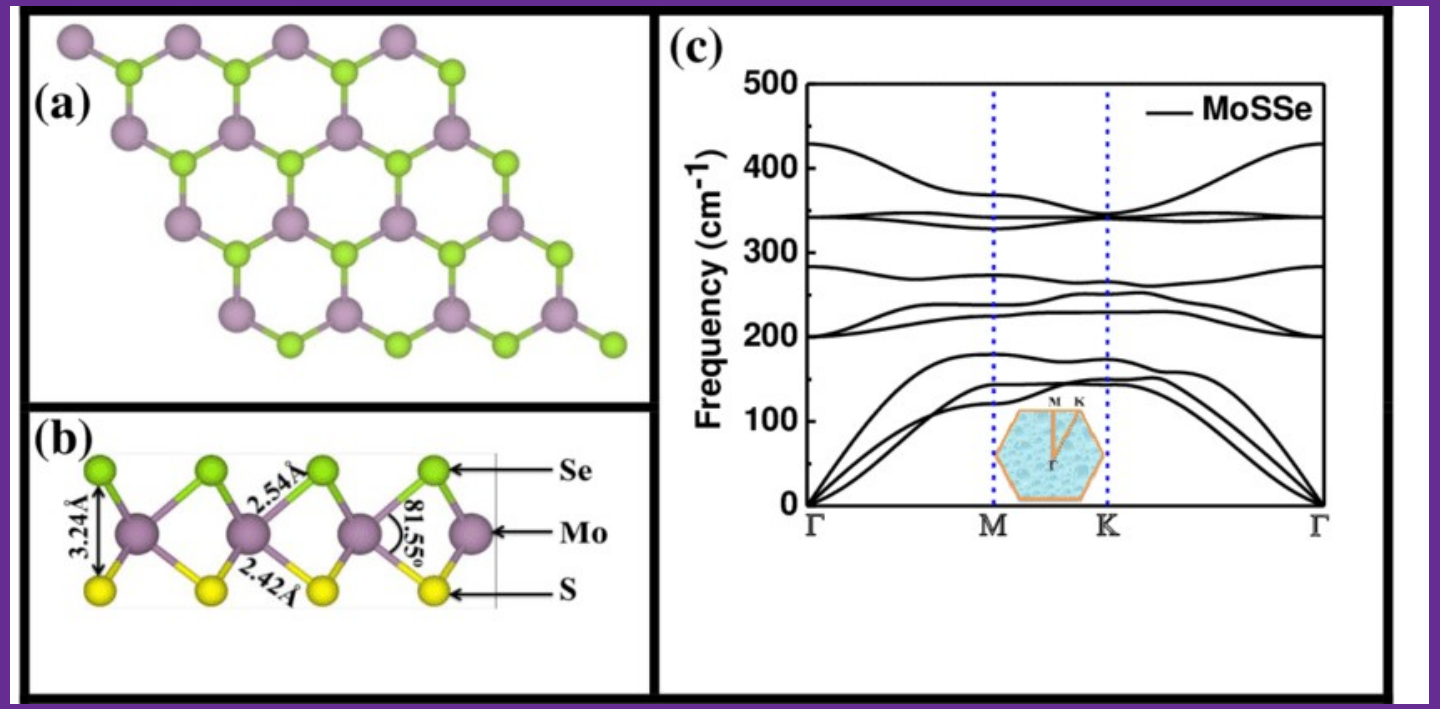
1. Faster electron hole recombination

2. Difficulty to achieve the desired morphology and need precise experimental techniques

3. For applicational purposes, we need hetero-junctions with other lattice matching semiconductors

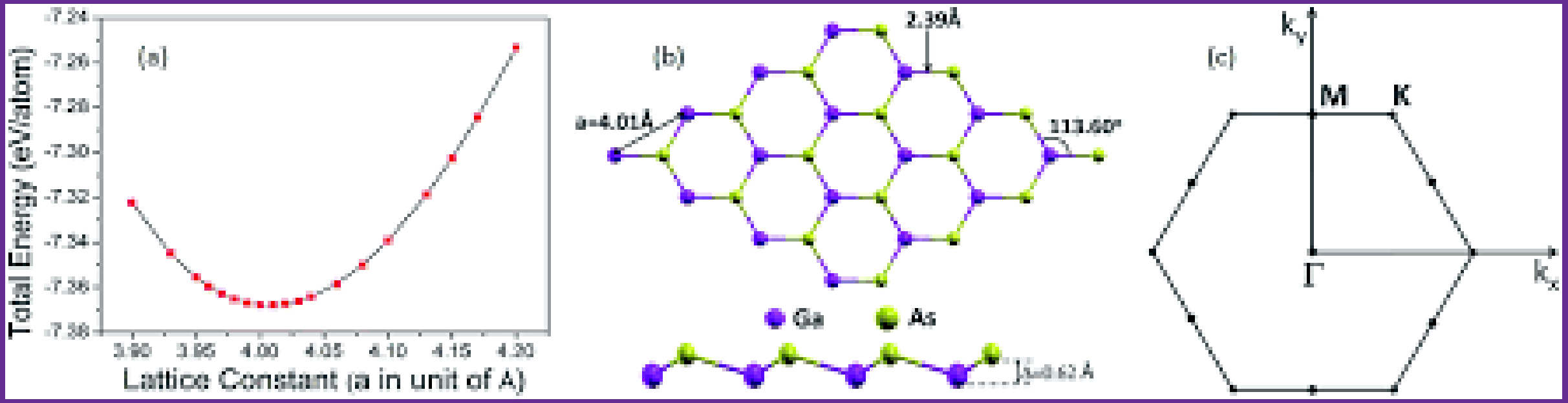
ACS Materials Lett. 2020, 2, 4, 336–357

MoSSe monolayer



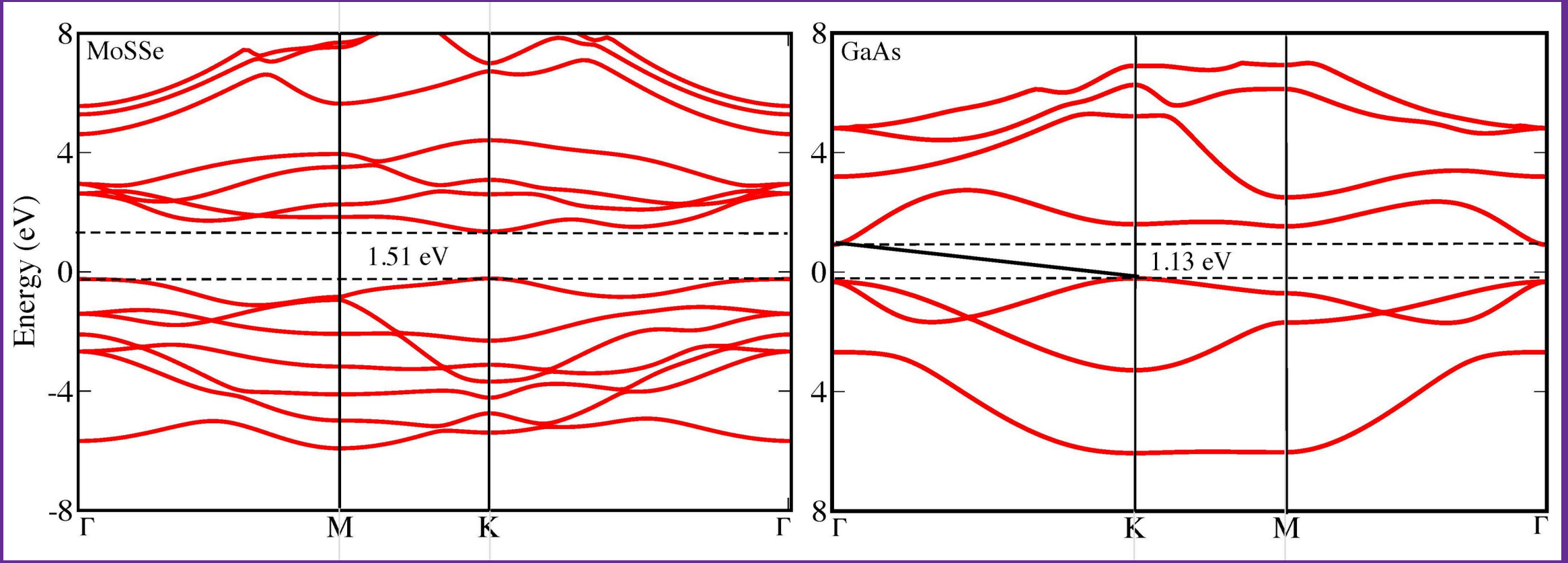
Applied Surface Science, Volume 490, 1 October 2019, Pages 204-219

GaAs monolayer



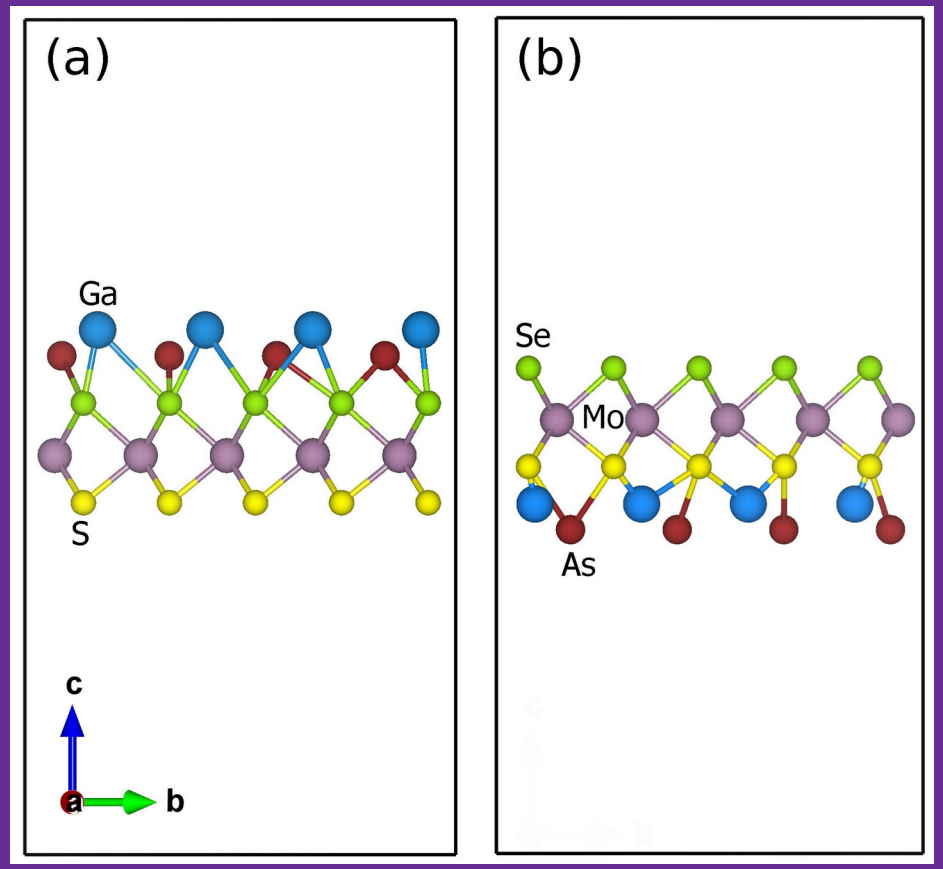
RSC Adv., 2016,6, 52920-52924

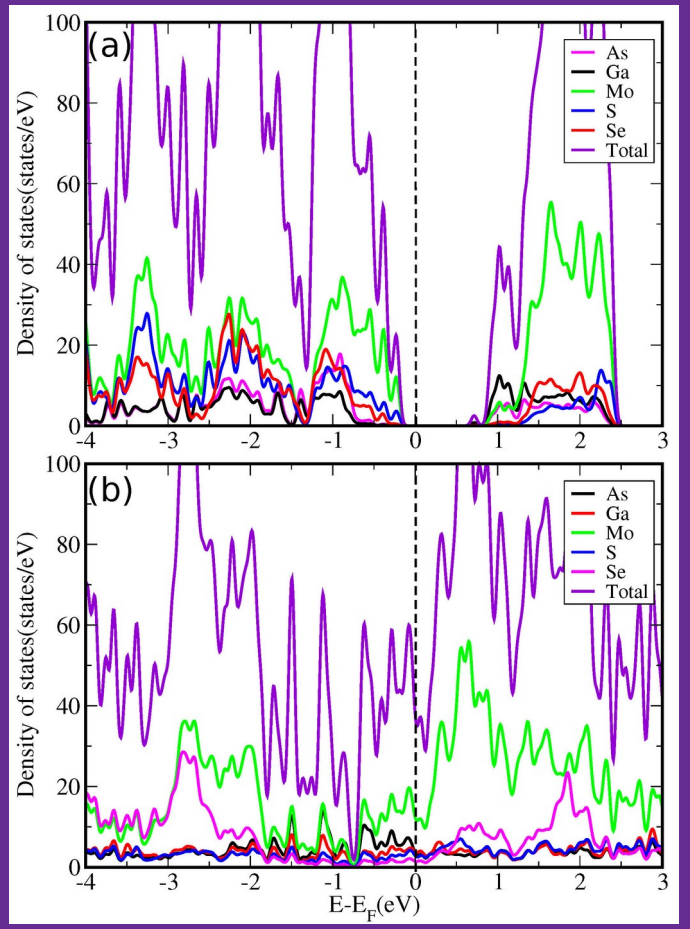
Electronic bandstructure of MoSSe and GaAs monolayers



Albar A, Aravindh SA. Emergence of metallic states at 2D MoSSe/GaAs Janus interface: a DFT study. J Phys Condens Matter. 2021 Sep 10;33(47). doi: 10.1088/1361-648X/ac2202. PMID: 34450605.

Janus/Semiconductor Heterojunctions





MoSSe-GaAs-IF-Se

MoSSe-GaAs-IF-S

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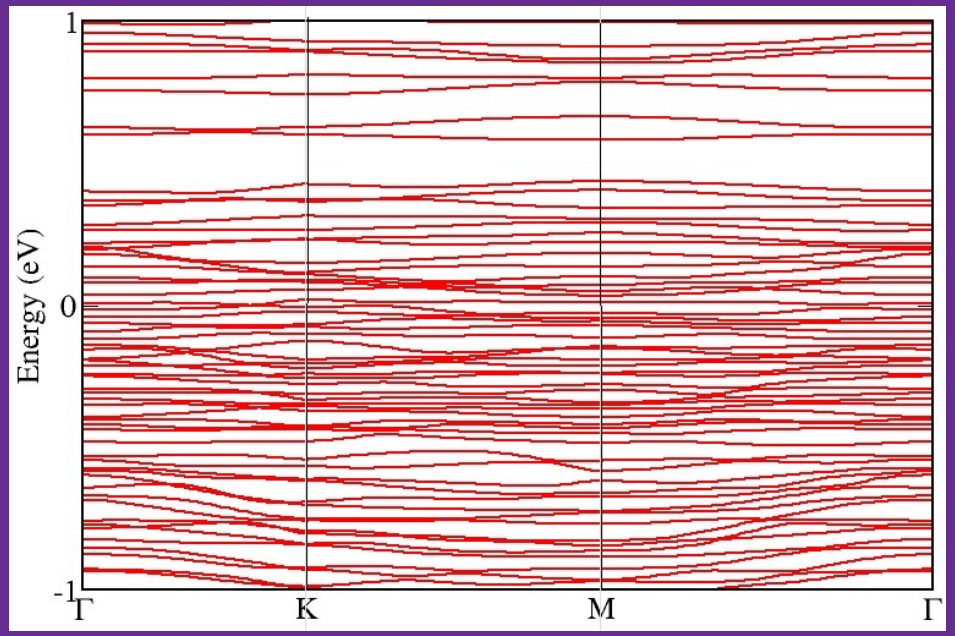
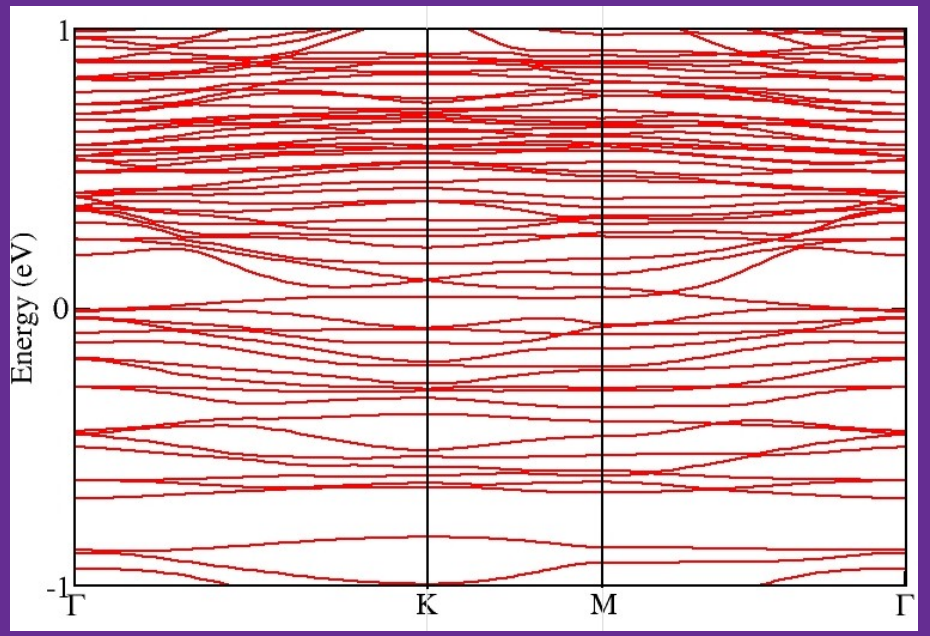
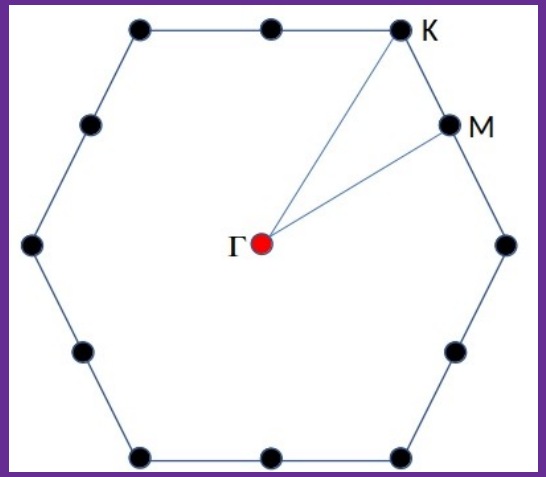
Electronic structure of Heterojunctions



MoSSe-GaAs-IF1



MoSSe-GaAs-IF2



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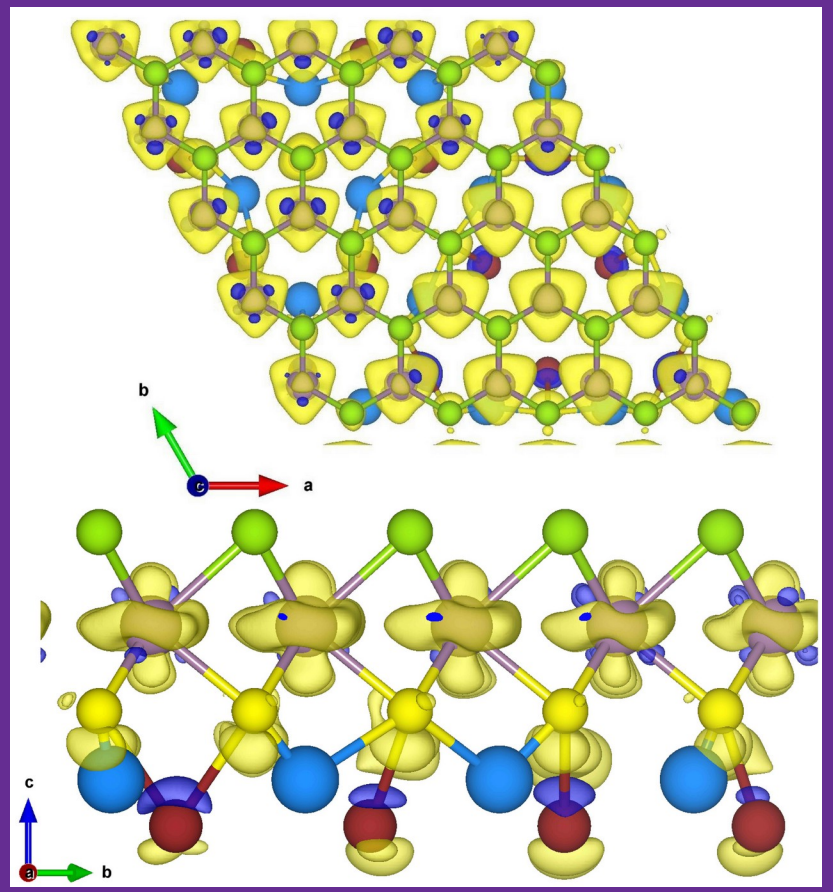
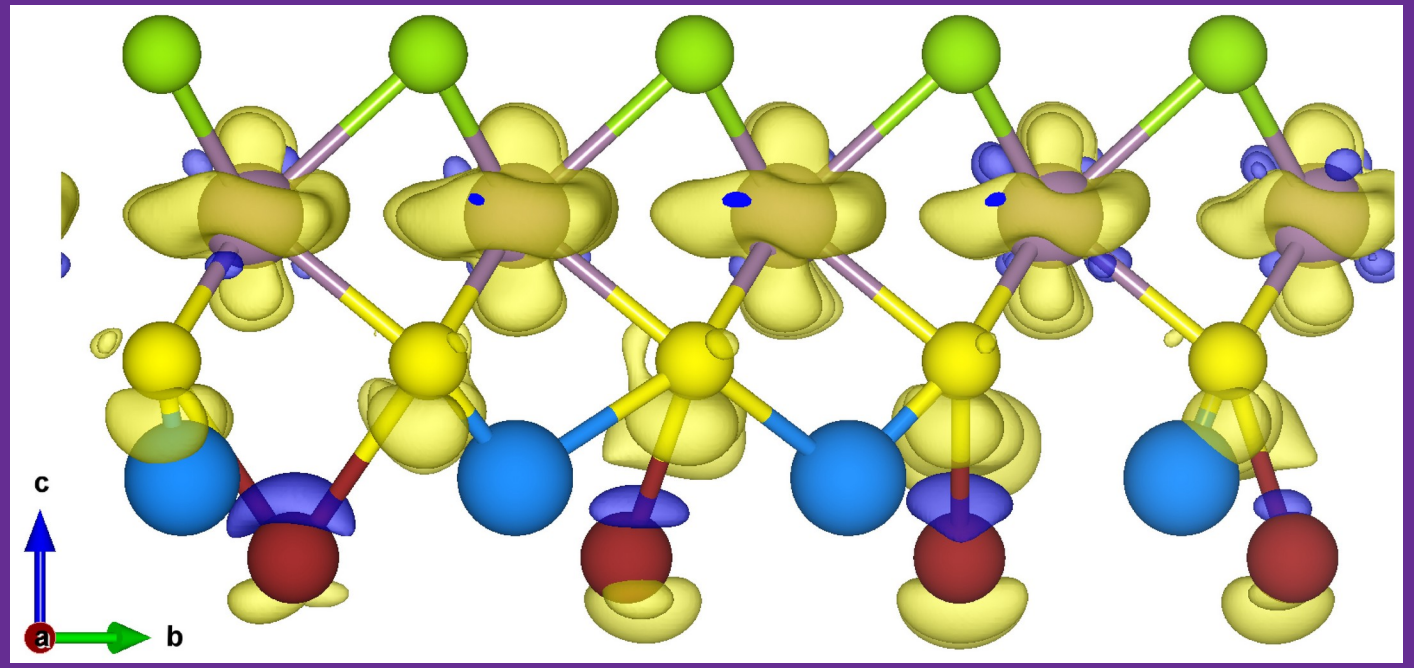
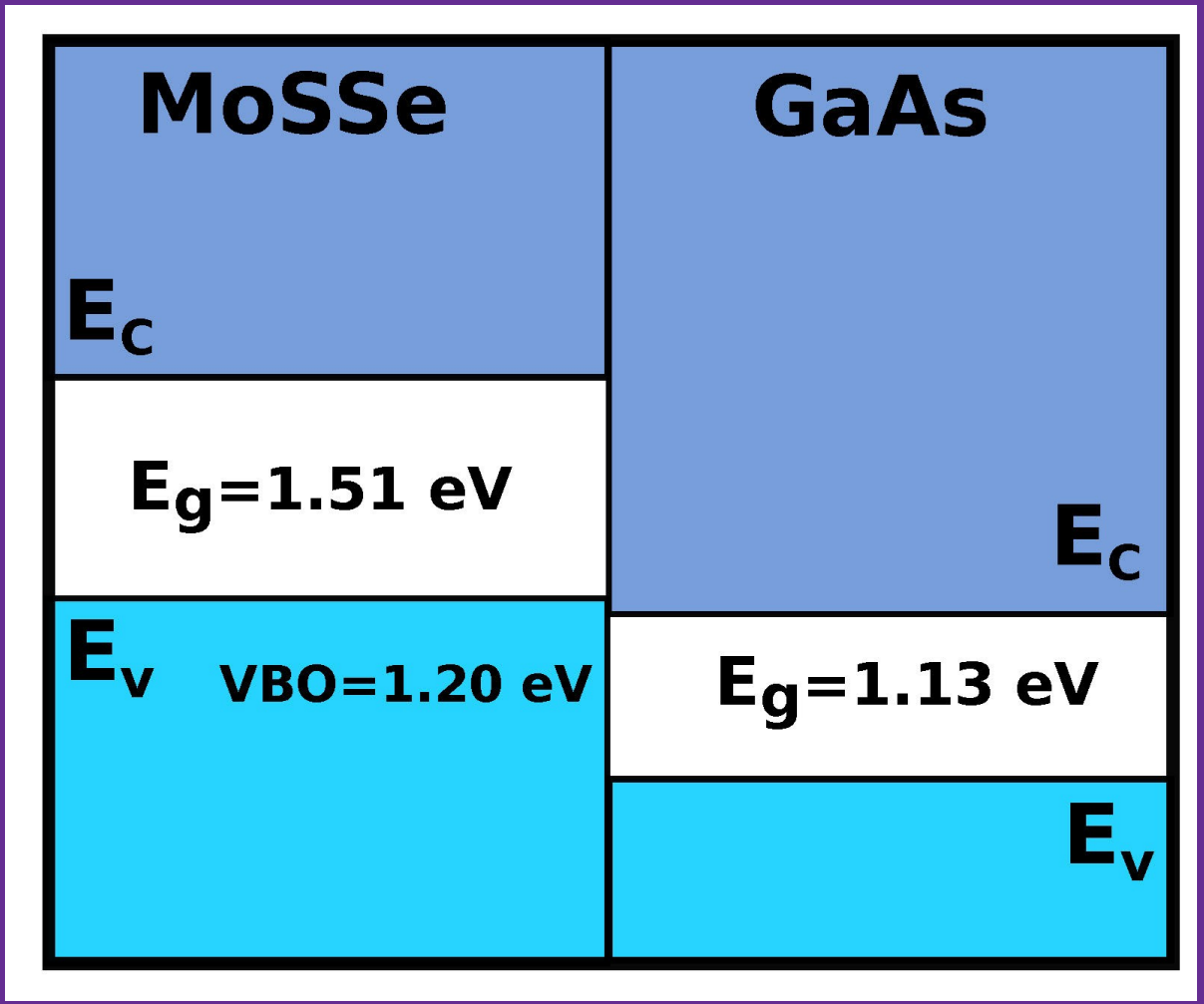
Charge density difference plot of the Heterojunctions





Top and side view of partial charge density difference plot for interface 2 of MoSSe/GaAs structure as specified in Figure 1. The bands are within an energy range −1 to 0 eV (with a value of 0.01 e/ ˚A3). Blue and yellow indicates electrons and holes, respectively

Band alignment diagram



BO = (EM oSSe + VM oSSe) −(EGaAs + VM oSSe) + ΔV

Where EMoSSe = −3.05 eV and EGaAs = −4.19 eV are the valence band maximum of bulk MoSSe and bulk GaAs.

VM oSSe = −6.66 eV and VGaAs = −3.80 eV, which are the macroscopic average electrostatic potentials for the bulk materials.

ΔV= 0.52 eV is the shift of the averaged electrostatic potential energies across the interface.

The obtained valence band offset is −1.20 eV.

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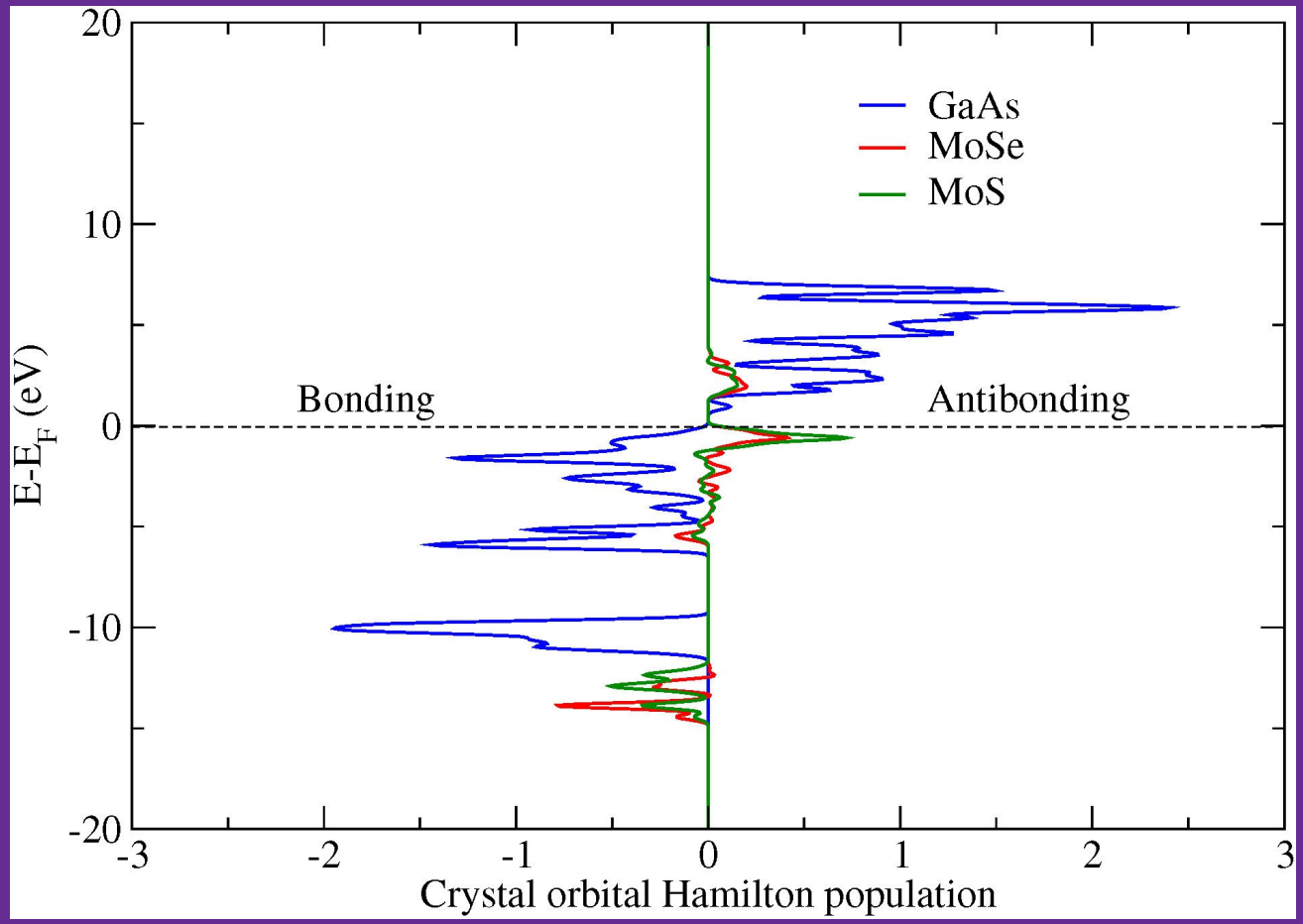
Crystal orbital Hamilton population



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Conclusions

A density functional theory study was undertaken to provide theoretical understanding of the electronic properties at 2D Janus GaAs/MoSSe interface.

Our investigation revealed the importance of interface atomic termination on the electronic and the structural properties of 2D Janus interfaces.

Metallic states were obtained only at the interface with MoS termination while the interface with MoSe termination is insulating and energetically not favorable.

Occupied antibonding states were found in MoSSe which drives the charge transfer from MoSSe to GaAs.

The calculated band alignment demonstrated the presence of charge transfer from MoSSe to GaAs, which is the reason for the metallic states at GaAs/MoSSe interface.

Our results indicate that the stability and electronic properties of 2D Janus interfaces are affected by the interface termination which is critical for practical applications

Acknowledgements

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Thank you for your attention