Tuning the electronic structure of Janus WSSe-ZnO heterostructures from first-principles

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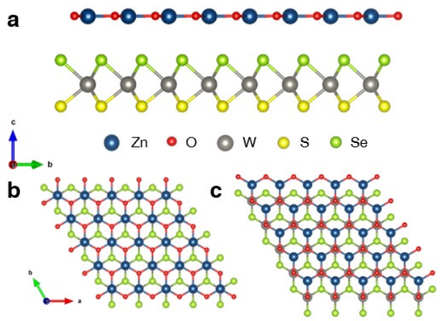
Abstract

- Two-dimensional (2D) materials, with their highly tunable electrical characteristics, are a new class of materials being explored for use in green energy technologies.
- While the photophysical properties of monolayer semiconducting 2D materials like transition metal dichalcogenides (TMDs) have been extensively studied for these applications, van der Waals (vdW) heterostructures made up of stacks of various types of 2D materials offer the opportunity to further tune and optimize the electronic properties of 2D materials.
- In this work we use density functional theory (DFT) calculations to study the electronic structure of a vdW heterostructure of Janus WSSe with the novel 2D material monolayer ZnO. The effects of alignment, strain, and electric field are investigated.



Why Van der Waals Hetrostructures

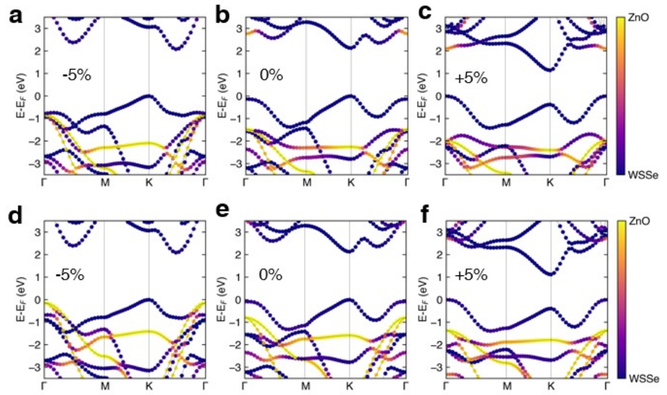
- Individual 2D materials only have a limited set of properties, limiting the development and use of 2D material devices.
- In the realm of materials discovery and design, van der Waals (vdW) heterostructures, which mix the properties of distinct monolayers to generate new materials with hybrid features, have recently gotten a lot of interest.
- We investigate the photocatalytic and photovoltaic characteristics of vdW heterostructures of the Janus TMD WSSe and monolayer ZnO. W-based TMDs have narrower band gaps and absolute band edge positions shifted to higher energy than Mo-based TMDs, improving their capacity to absorb a substantial portion of the visible spectrum and having conduction band edges at high enough energies to contribute electrons for photocatalytic reduction. Janus TMDs also contain built-in electric fields that can help with charge separation.

Methods

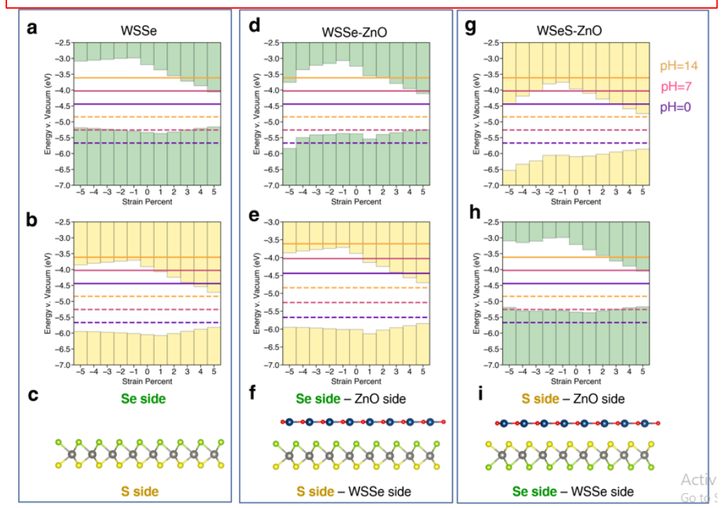
- **Density functional theory as implemented in VASP and QE code.**
- **Materials studio**

Results

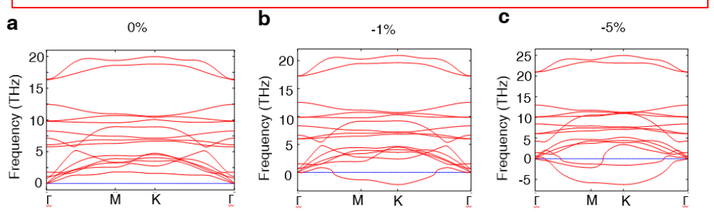
Band structures of the Janus TMD-ZnO heterostructures for WSSe-ZnO (a,b,c) and WSeS-ZnO (d,e,f) at 5% compressive strain (a,d), no strain (b,e), and 5% tensile strain (c,f).



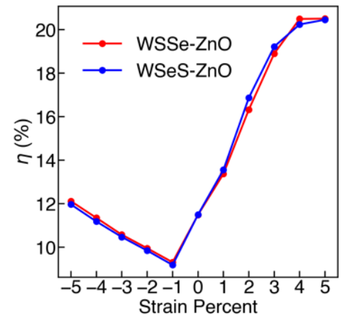
Schematics of band edge alignments under in-plane biaxial strain



Phonon band structures of the WSeS-ZnO heterostructure under (a) 0% (b) 1% and (c) 5% in-plane biaxial compressive strain



Power conversion efficiency of the two stable Janus TMD-ZnO configurations



Conclusions

- The effects of in-plane biaxial strain, out-of-plane uniaxial strain (vertical proximity), and electric field on the electronic structure of Janus WSSe-ZnO heterostructures were studied using DFT calculations, with the goal of optimizing their electronic properties for photocatalytic and photovoltaic applications.
- In general, if the PZC of these heterostructures were reached under acidic conditions, the S side of these heterostructures is preferable for straddling the HER and OER potentials. Under neutral conditions either side has band edge energies that are appropriate for the catalytic surface. Under basic conditions, the Se side of these heterostructures is generally preferable.
- For photovoltaic applications, the band gap reduction increases the potential power conversion efficiency up to an upper bound of 20% which makes the system very promising for solar cell applications.
- Our research on Janus WSSe-ZnO heterostructures shows that strain can be used to tune the band gaps and absolute band edge energies of vdW heterostructures of 2D materials with finite dipole moments, an effect that should be generalizable to other vdW heterostructures, making them exciting new candidates for photocatalytic and photovoltaic applications.

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