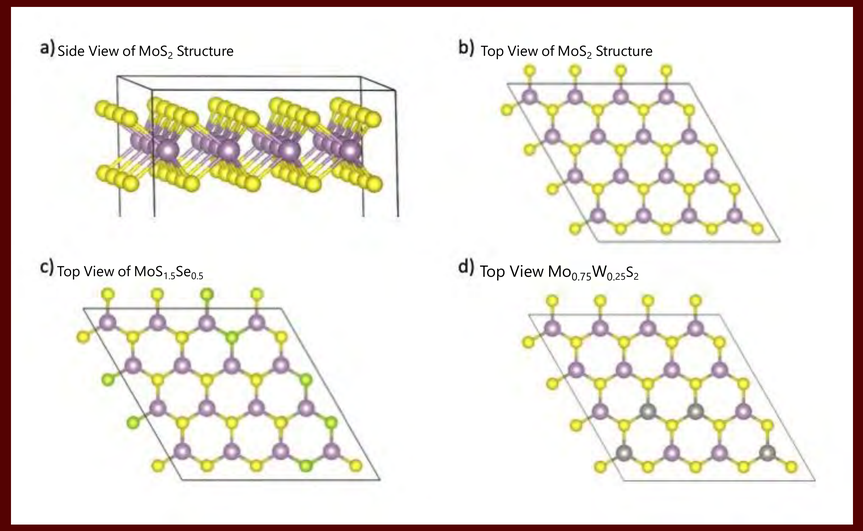
Effects of strain engineering on the optoelectronic properties of alloyed two-dimensional transition metal dichalcogenides.



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Introduction and Methods

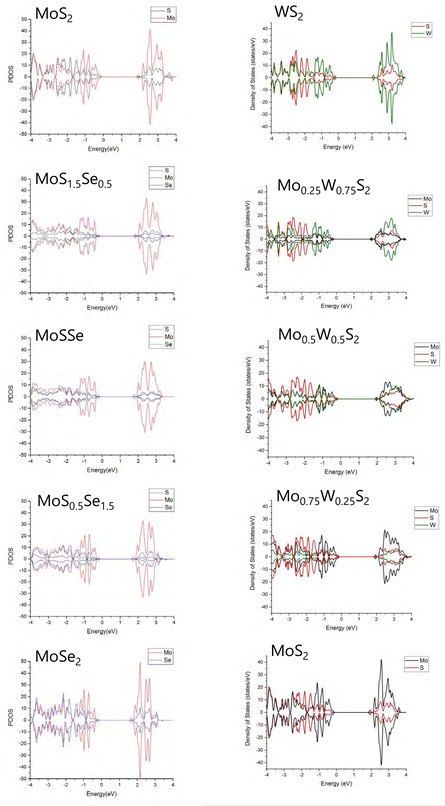
- Two-dimensional (2D) transition metal dichalcogenides (TMDs) are attractive semiconductors for use in electronic, optoelectronic, and spintronic devices
- Optoelectronic properties can be tuned by alloying and strain

- Alloys: $Mo_xW_{(1-x)}S_2$ and $MoS_{2x}Se_{2(1-x)}$
- Concentrations ranging from 0-100%
- Tensile and compressive strains ranging from 0-10%

- Density functional theory (DFT) used to:
  - Analyze the equilibrium structure
  - Derive the band gap
  - Examine the electronic structure at the varying levels of concentration and strain

PDOS (Projected Density Of States)

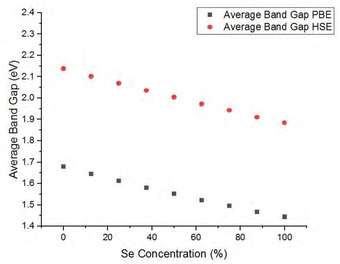
For $MoS_{2x}Se_{2(1-x)}$ and $Mo_xW_{(1-x)}S_2$, the alloy concentration changes the alloyed elements' contribution to the density of states, but the metal/chalcogen makeup of the band edges remains mostly the same.



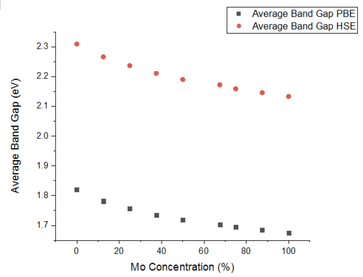
Unstrained Alloys' Band Gaps

For $MoS_{2x}Se_{2(1-x)}$, the band gap decreases with increasing Se concentration. For $Mo_xW_{(1-x)}S_2$, the band gap decreases with increasing Mo concentration.

$MoS_{2x}Se_{2(1-x)}$



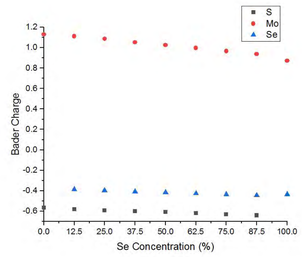
$Mo_xW_{(1-x)}S_2$



Unstrained Alloys' Bader Charge

For $MoS_{2x}Se_{2(1-x)}$, as Se concentration increases, Bader charges of S and Se remain consistent, and charge transfer from Mo decreases.
For $Mo_xW_{(1-x)}S_2$, as Mo concentration increases, Bader charges of Mo and W remain consistent, while charge transfer to S slightly decreases.

$MoS_{2x}Se_{2(1-x)}$



$Mo_xW_{(1-x)}S_2$