Two-Dimensional Electronic Materials: Transition Metal Dichalcogenides (TMD)

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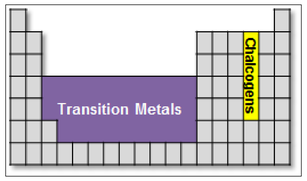
1. Background

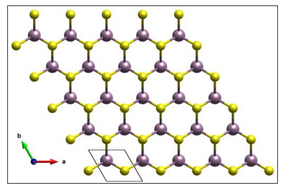
Transition Metal Dichalcogenides (TMDs)

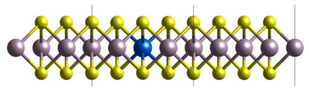
- Two-dimensional materials with improved properties when transitioning from bulk (3D) to monolayer (2D)
- Chemical formula of type MX_2
  - M = transition metal
  - X = chalcogen
- Many properties of TMDs are reminiscent of graphene
  - Many TMD compositions have **band gaps**, but graphene has a zero band gap

Motivation

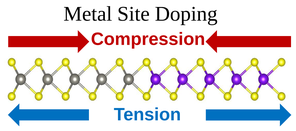
- Understanding how to tune the electronic band gap of TMDs
  - Metal site doping
  - Tensile and compressive forces
- Understanding interfacial thermal transport







Metal Site Doping

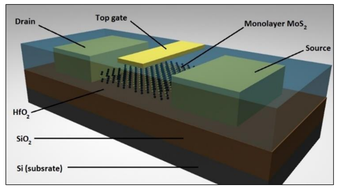


Strain on Heterostructures

2. Practical Applications

High-Performance Electronics

- Field effect transistors (FETs)
  - Due to the presence of a band gap, many TMD compositions can be used as semi-conductors in the next-generation of FET technology.
  - TMDs have a high electron mobility when compared to Si.



Model of an FET[1]

- Flexible/wearable electronics
  - TMDs are relatively strong and flexible.
  - Some compositions are semi-transparent.
  - These unique properties make TMDs very intriguing for use in flexible and wearable technology.
- Optoelectronics
- Energy storage
  - TMDs can also be used as the anode in lithium ion batteries

3. TMD Heterostructures

Types of Heterostructures

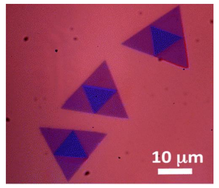
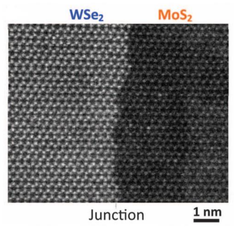
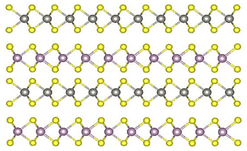


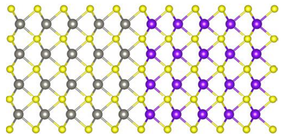
Image of MoS_2-WSe_2[2]



STEM Image of MoS_2-WSe_2[3]



Vertical Structure



Lateral Structure

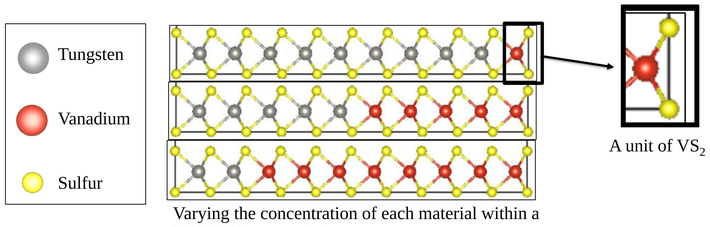
- Lateral heterostructures
  - Held together by strong covalent bonds
- Vertical heterostructures
  - Held together by weak Van der Waals forces

Materials-by-Design

- The ability to mix-and-match different TMDs allows the creation of devices that can be designed to meet highly specific requirements for a task.

Varying Concentration

- We have studied how the concentration of each material affects the properties of the system, as shown below.



Varying the concentration of each material within a MX_2-MX_2 composition

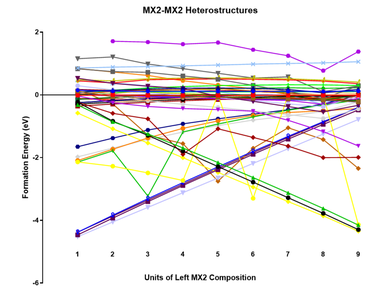
A unit of VS_2

4. Methods

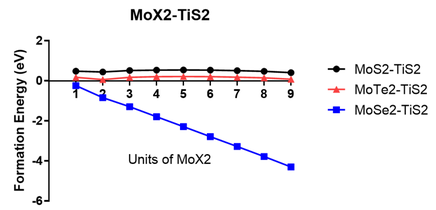
Density Functional Theory (DFT)

- DFT is an electron-density-dependent method.
  - Ground-state properties of a many-body electron system are only a function of electron density.
- We used the Vienna Ab initio Simulation Package (VASP) to perform our DFT calculations.
  - Using DFT methods we could optimize TMD heterostructures and attain their formation energies.

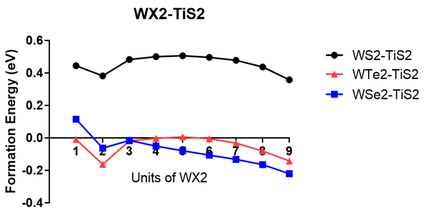
5. Preliminary Results



- Over 500 MX_2-MX_2 formation energies were found using DFT calculations.
  - The formation energies of these structures are all plotted in the figure to the left
  - Analysis of data is a work in progress



- We isolate one of the X_2 variables to understand how the choice of chalcogen effects the formation energy of the composition.



- Preliminary data suggests that a greater abundance of Se correlates with a lower formation energy, followed by Te, and then finally S.
  - The cause of this trend is currently unknown.

6. Conclusion/Future Work

- A thorough and proper data analysis is needed before we draw any solid conclusions.
- In this study we focused on the formation energy and structural stability of MX_2-MX_2 compositions. Future studies will involve calculating the band gap as a function of composition.

Acknowledgements

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3. Epitaxial growth of a monolayer WSe2-MoS2 lateral p-n junction with an atomically sharp interface. M. Y. Li, Y. Shi, C. C. Cheng, L. S. Lu, Y. C. Lin, H. L. Tang, M. L. Tsai, C. W. Chu, K. H. Wei, J. H. He, W. H. Chang, K. Suenaga, and L. J. Li. (2015).