Two-Dimensional Transition Metal Dichalcogenides (2D-TMDs) Studies via Computer Calculations

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Abstract

The research work behind Two-Dimensional materials, such as Graphene opens a new set of possibilities to the creation of these type of materials that will have the same or even better thermoelectrically properties than Graphene. The main example of these materials, are the two-dimensional transition metal dichalcogenides (2D-TMDs), which in this case we'll be working with MoS_2. This molecule, will then be doped or assembled in a vertical heterojunction with semiconductors; to later measure the interaction between the atoms in both process. Our objective is to develop, via computational calculations (VASP), the most stable and efficient set of atoms and their ground state; that in the future could end up having very useful technological applications, such as sensors, communication systems, intelligent memory and much more.

Background

- **2D-TMDs**
  - Also known as MX2s

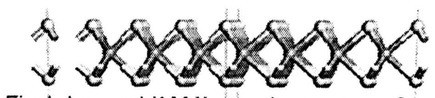
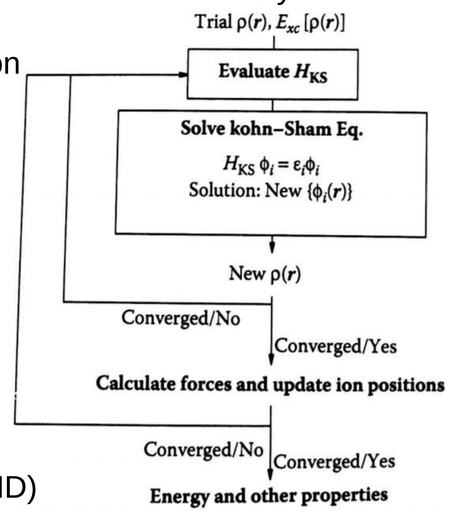


Fig 1. Layered X-M-X atomic structure of MX_2 along c-axis. M is shown in blue, and S in yellow. Adjacent layers (not shown) form with weak van der Waals interactions.

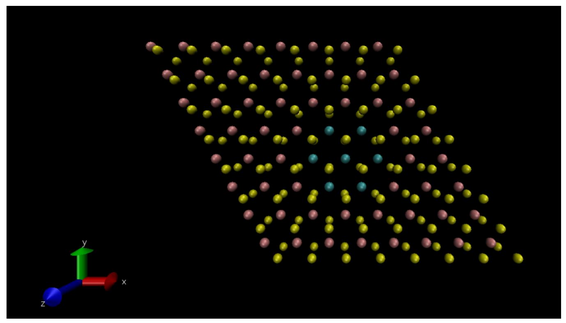
- **VASP**
  - The software code use to calculate DFT calculations

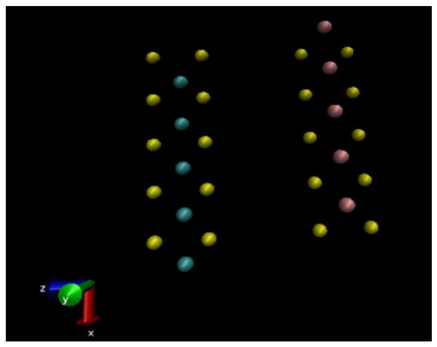
Methods & Procedure

- First-principles of Density Functional Theory (DFT)
  - For Geometry Optimization Calculations
- Convergence Test
  - In order to find the ideal Ground State Energy



- Creating the Molecules (VMD)
  - Increasing the dopance (Ti) concentration
  - Assembling a vertical Heterojunction (W)





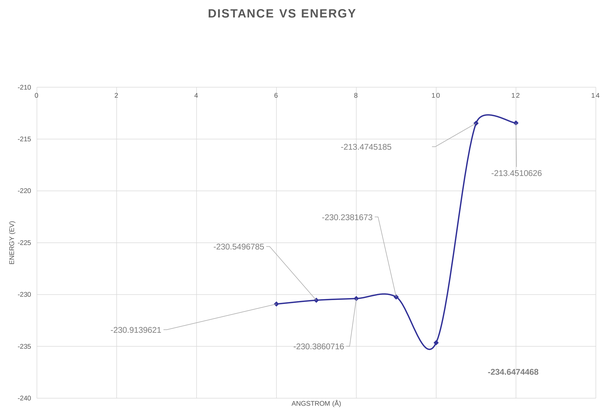
Results & Conclusion

- Doping (Ti)

$$E_{Total} - E_{Pure} - E_{Ti} = E_{Formation}$$

Tiatoms	Etotal	Epure	Eti	Eformation
1	-1391.712272	-1394.895482	-2.29388	5.4770896
2	-1388.803897			10.6793448
3	-1385.99911			15.77801203
4	-1383.538026			20.53297547
5	-1380.695771			25.66911022
6	-1378.212942			30.44581935
7	-1375.728345			35.22429652

- Vertical Heterojunction (W)



Although the atoms in the molecules interacted in a great way between each other, further analysis needs to be done, like increasing the doping concentration and assembling new vertical heterojunctions with other semiconductors, to understand better the thermoelectric properties of these materials.

Cao, Z., Harb, M., Lardhi, S., & Cavallo, L. (2017). Impact of Interfacial Defects on the Properties of Monolayer Transition Metal Dichalcogenide Lateral Heterojunctions. *The Journal Of Physical Chemistry Letters*, *8*(7), 1664-1669. http://dx.doi.org/10.1021/acs.jpclett.7b00518

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