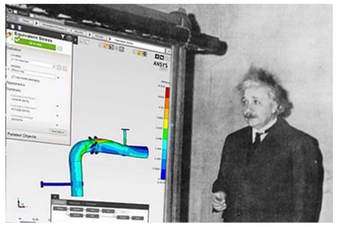
Electronic and Thermoelectric Characterization of Materials from Ab Initio Calculations

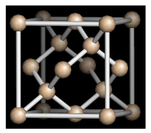
Gustavo Javier-Rico[1], Austin Zadoks[2], David M. Guzman[2], and Alejandro H. Strachan[2]

[1]Department of Physics, California State University of Los Angeles [2]School of Materials Engineering and Birck Nanotechnology Center Purdue University, West Lafayette IN

Motivation

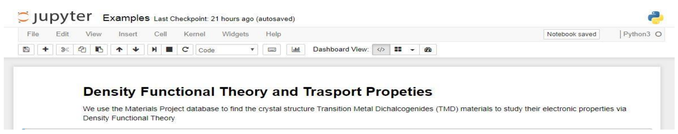
- Ab-Initio calculations are a powerful aid to both theoretical and experimental scientists to better understand electronic structure and materials design.
- Performing Ab-Initio calculations can be a convoluted process. This work aims at simplifying the interaction between researchers and databases/Ab-initio simulation engines.

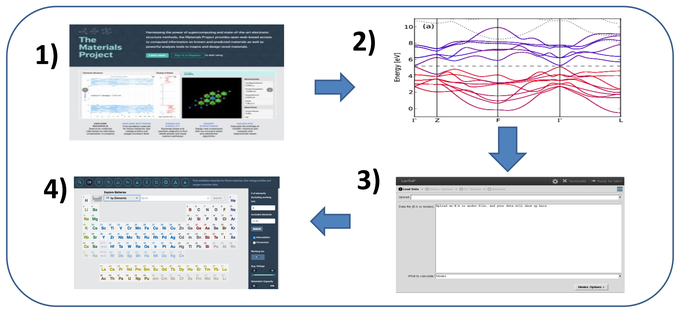




Workflow

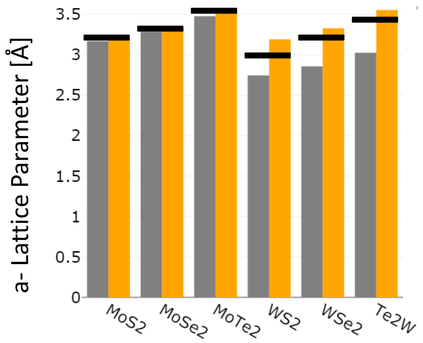
The **O**ptimized **W**orkflow for **E**lectronic and **T**hermoelectric **P**roperties **(OWETP)** invokes the functionalities of the following tools.

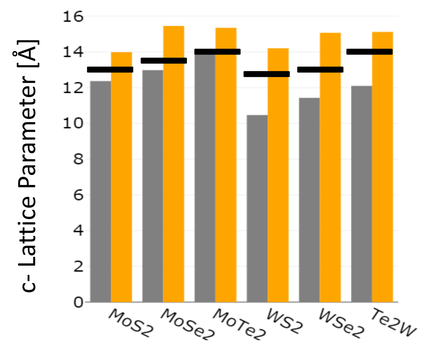


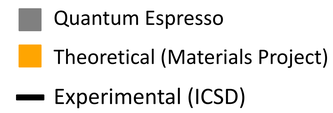


1) The Materials Project (MP) Database on the web
2) Band structure calculations with Density Functional Theory implemented in the Quantum Espresso code
3) Landauer Transport Properties (LanTrap) with the Landauer-Datta-Lundstrom generalized transport method.
4) Materials Project theoretical/experimental results database

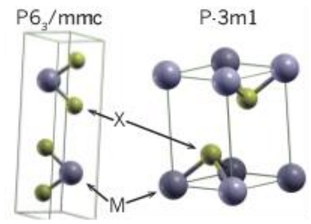
Application I – Structural Properties of Transition Metal Dichalcogenides (TMDs)

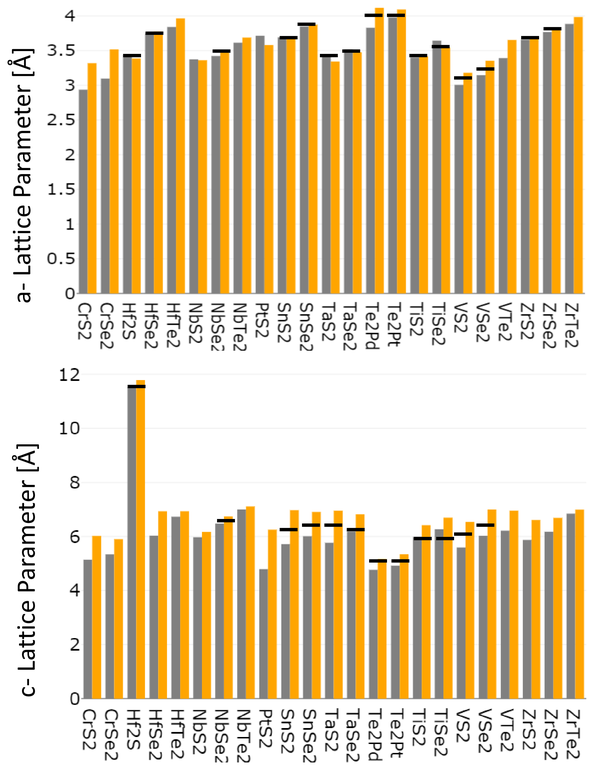






- These TMDs are also classified as Van Der Waals materials due to their atomic layered structure. They belong to space group $P6_3/mmc$ or P-3m1
- The OWETP python notebook's predictions for lattice parameter characterization are consistent with both theoretical and experimental results, as compared with the Materials Project and ICSD database.





OWETP's road map to thermo-electric calculations:

Query MP database for material of interest

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Perform band structure calculations.

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Parse output files to be LanTraP compatible

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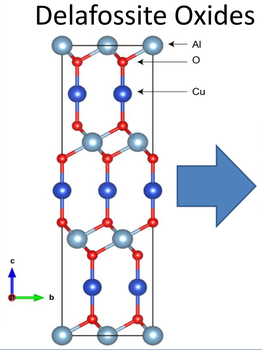
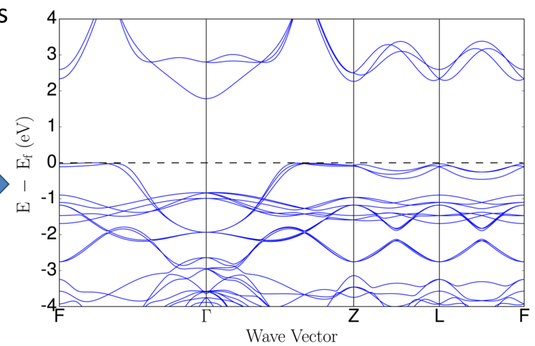
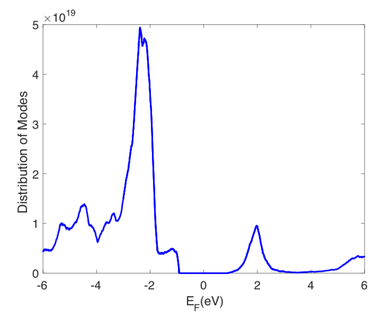
Connect to LanTraP

Application II – Thermoelectric Properties

Delafossite Oxides







Conclusion

Ab Initio simulation methods may not be available to scientists due to the complexity of their infrastructure. In this effort, we offer to bridge that gap and encourage both theoretical and experimental scientists to explore the predictive power of these tools. The OWETP python notebook offers a straight forward, more accessible way to carry out simulations from first principle's theory

References

[1] Guzman, M. David,. Strachan, "Role of Strain on Electronic and Mechanical Response on Semi-Conducting Transition Metal Dichacogenides Monolayers," "*Journal of Applied Physics*", Volume 2014, Article ID 243701
[2] Conrad, Kyle,. Maassen, Jesse., and Lundstrom, Mark(2014)., "LanTraP," https://nanohub.org/resources/lantrap. (DOI: 10.4231/D3NP1WJ64).
[3] Kruglyak, Yuriy,, "Landauer-Datta-Lundstrom Generalized Transport Model for Nanoelectronics," *Review Article* , Volume 2014, Article ID 725420

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