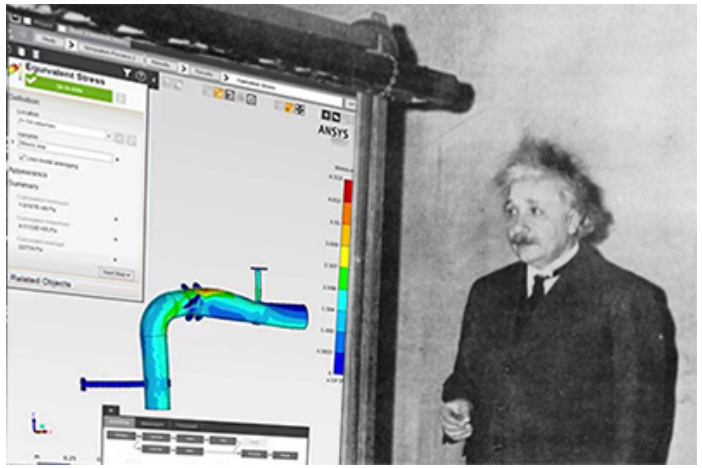
Electronic and Thermoelectric Characterization of Materials from Ab Initio Calculations



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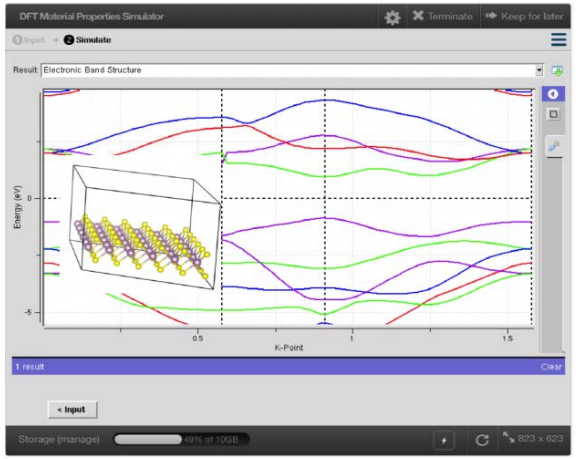
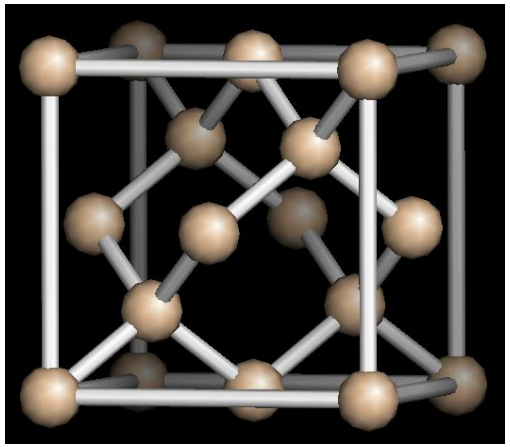
NCN-URE 2017
Strachan Group

Objectives

- Motivation: Ab Initio Simulation Tools are Awesome
- Introducing OWETP
- Case Study I: Structural Properties of TMDs
- Case Study II: Thermoelectric Properties of Silicon
- Future Work

Motivation





- Simulation Tools Provide insight into the structure of materials
- They can corroborate experimental data

Experiment

+

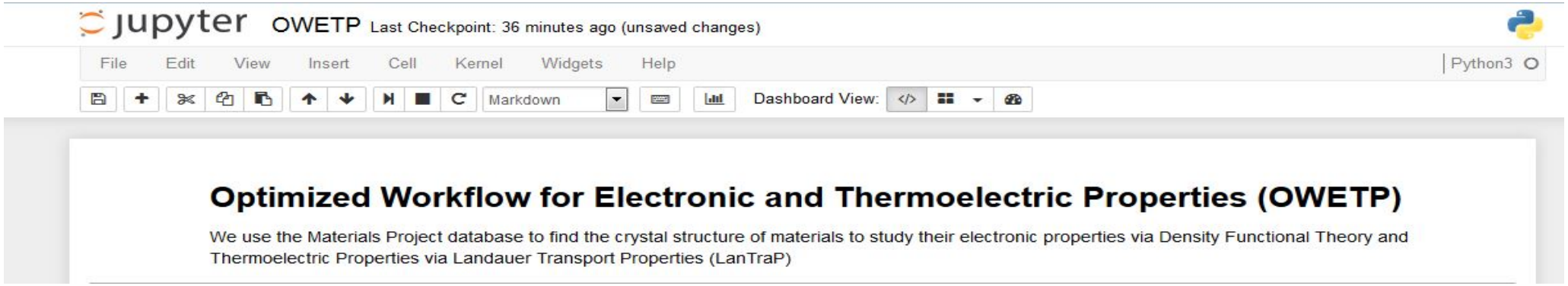
Simulation

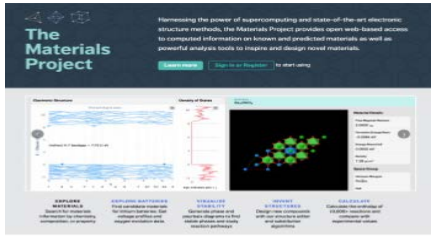
=

Reliable Results

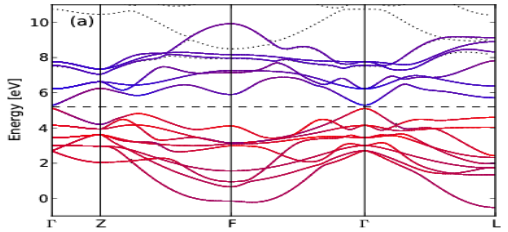
OWET nanoHUB Simulation Tool

(Optimized Workflow for Electronic and Thermoelectric Properties)

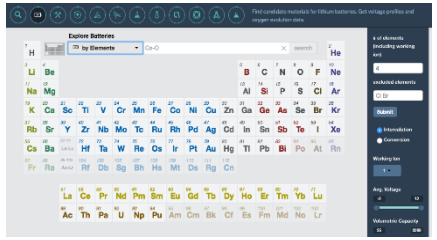




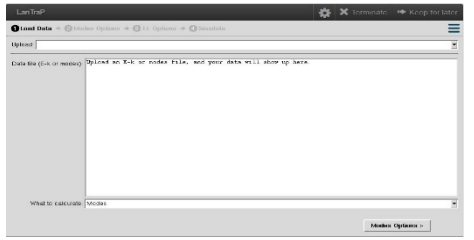
Material Project Database



Electronic Structure



ICSD via Materials Project

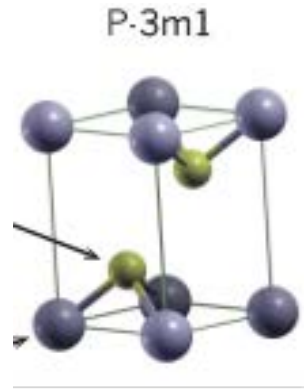


LanTraP nanoHUB tool

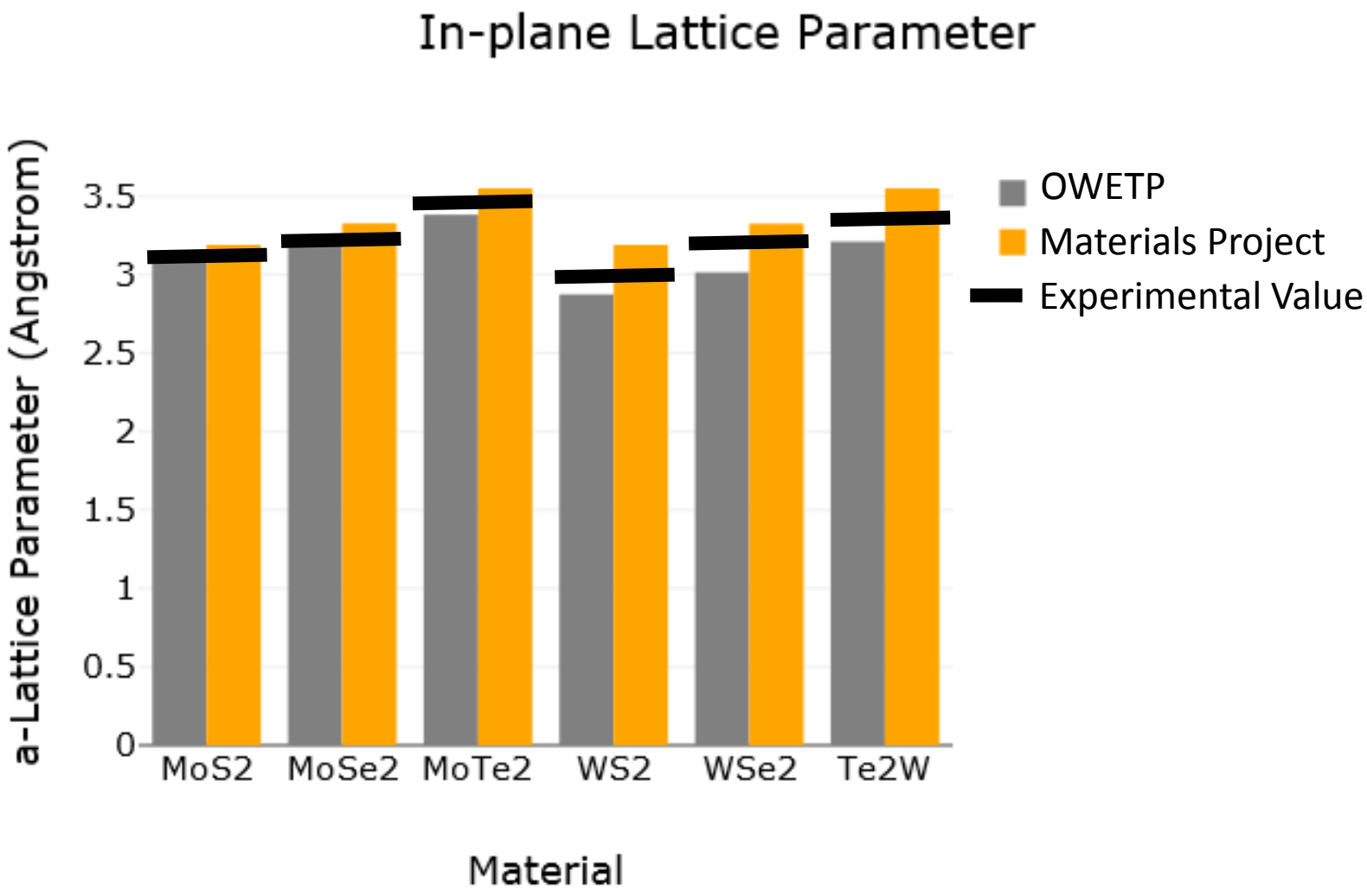
Connect to the Materials Project Database

Define Query Criteria, Connects To Materials Project Database, and Submits Jobs

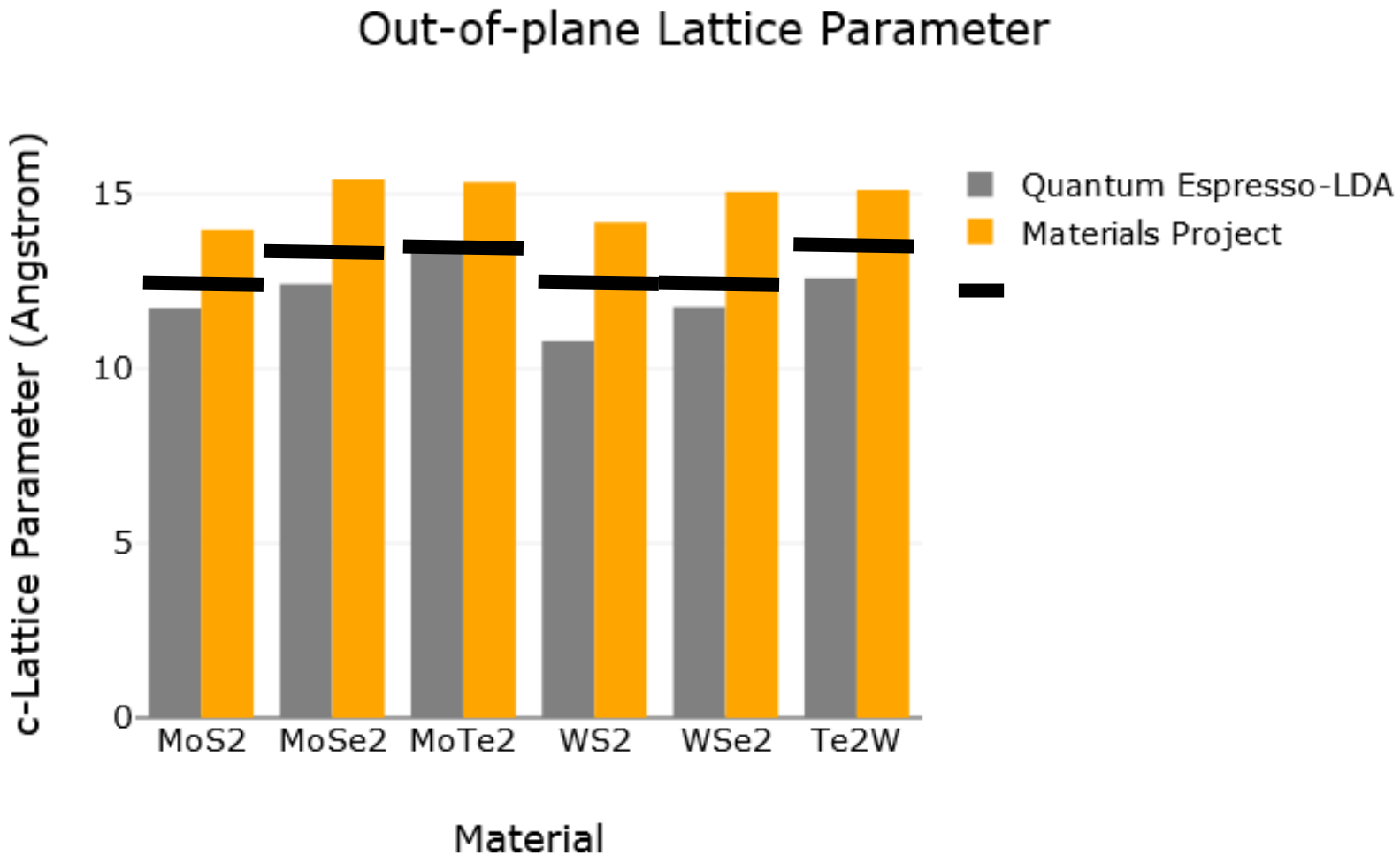
In [78]:
```
criteria1 = {
    "spacegroup.symbol":     "P6_3/mmc",
    "nelements":             2,
    "nsites":                6,}
criteria2 = {
    "spacegroup.symbol":     "P-3m1",
    "nelements":             2,
    "nsites":                3,}

#Then, we define properties we want to retrieve from the matching materials
properties = [
    "spacegroup.symbol",
    "pretty_formula",
    "full_formula",
    "structure.lattice",
    "task_id",
    "elements",
    "final_energy",
    "e_above_hull",
    "cif",
    "input.incar",
    "input.crystal.sites",
    "icsd_ids",
    "run_type",
    "structure"
]
```



Case Study I: Structural Properties of Transition Metal Di-chalcogenides (TMDs)



Case Study I: Structural Properties of Transition Metal Dichalcogenides (TMDs)



Thermoelectric Ab Initio Calculations via LanTraP

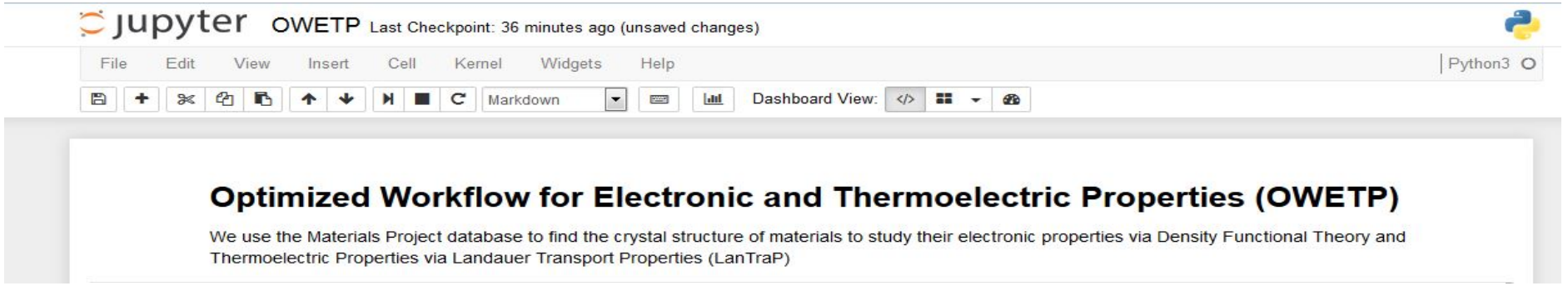
BAND STRUCTURES
(Via Density Functional Theory)

DENSITY OF MODES
(Via Landauer-Datta- Lundstrom)

THERMOELECTRIC METRICS

Kruglyak, Yuriy., "Landauer-Datta-Lundstrom Generalized Transport Model for Nanoelectronics," *Review Article ,* Volume 2014, Article ID 725420

Case Study II: Thermoelectric Properties of Silicon



Connect to Materials Project database and define criteria for Silicon

In [90]:
```
criteria = {
    "task_id":     "mp-149",
        }
properties = [
    "spacegroup.symbol",
    "pretty_formula",
    "full_formula",
    "structure.lattice",
    "task_id",
    "elements",
    "final_energy",
    "e_above_hull",
    "cif",
    "input.incar",
    "input.crystal.sites",
    "icsd_ids",
    "run_type",
    "structure"
]
key = "8DLSFHMP5zwaWhnT"
# This line conducts the query using a wrapper function
# built into this tool


Si_data=[]
Si_data.extend(mp_query(key,criteria = criteria,
               properties = properties))
```

```
connecting to the Materials Project ...Connected!
```

Quantum Espresso Input Files

In [49]:

```
control = {
        "calculation"                   :    "scf",
        "restart_mode"                  :    "from_scratch",
        "prefix"                        :    "scf",
        "verbosity"                     :    "high",         #"Low",
        "outdir"                        :    "./tmp" ,       #"./tmp",
        "forc_conv_thr"                 :    0.0002,
        "pseudo_dir"                    :    "./" ,
}

system = {
        "ecutwfc"                       :    30.00,
        "occupations"                   :    "smearing",
        "degauss"                       :    0.0038,
        "smearing"                      :    "gauss",

}

electrons = {
        "diagonalization"               :    "david",
        "mixing_mode"                   :    "plain",
        "electron_maxstep"              :    500,
        "conv_thr"                      :    1.0E-8,
        "mixing_beta"                   :    0.70,
}

ions = {
        "bfgs_ndim"                     :    1,
```

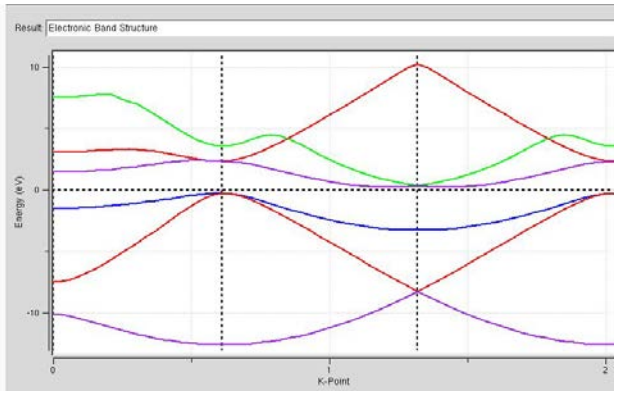
VC Relax

Self Consistent Field (scf)

Non-Self Consistent Field(nscf)

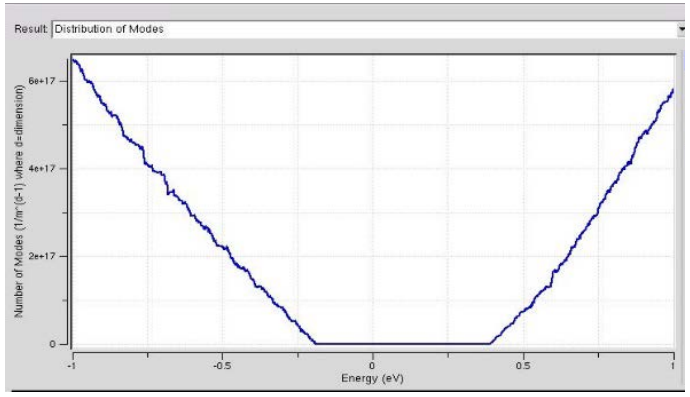
Bands

Case Study II: Thermoelectric Properties of Silicon

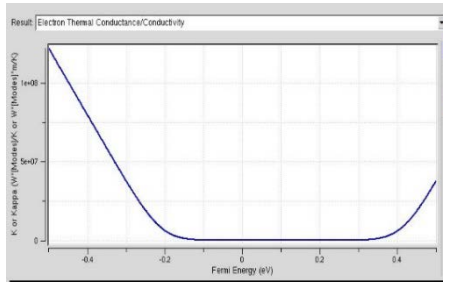


Band Structure

Call LanTraP

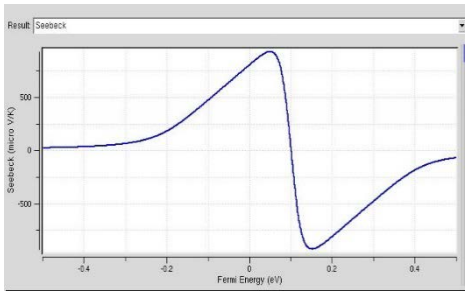


Density of Modes



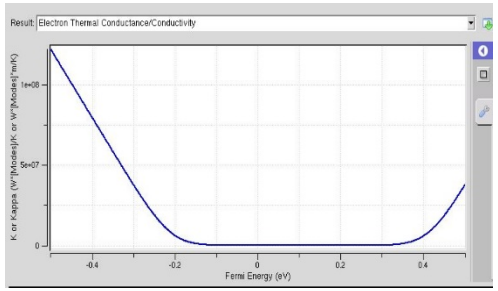
Electrical Conductivity

σ



Seebeck Coefficient

S



Electronic Thermal Conductivity

κ

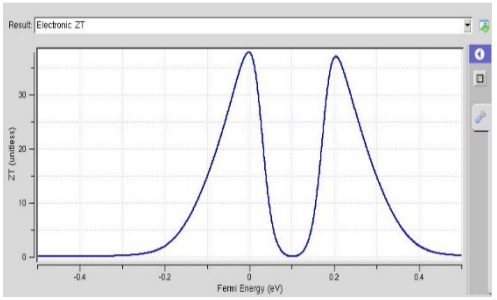


Figure of Merit

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Future Work

- We Would like to extend to the case of phonons in our thermoelectric study.

- Include examples of monolayers and more complicated structures.

- We would to be able to connect to more nanoHUB tools

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.

Acknowledgements

- I am very grateful to Professor Ale Strachan.
- All the member of the Strachan group, very especially David Guzman and Austin Zadoks.
- NCN, very especially Tanya Faltens and Ashley Byrne.
- The nanoHUB technical support team, Derrick Kearny, Martin Hunt, and Steve Clark.
- The physics department at California State University of Los Angeles.