Modeling Electronic Properties of Correlated Materials Using First Principles

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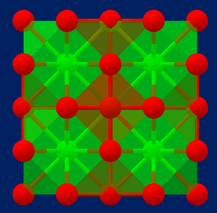
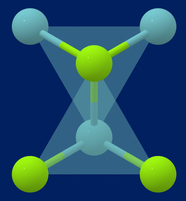
Materials

$SrVO_3$ (Cubic)



- Optically Transparent
- Conductive
- Tunable Electron Mobility

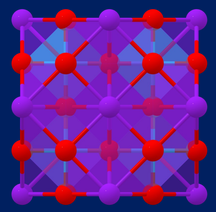
$NbSe_2$ (Hexagonal)



- Ferromagnetic
- Charge Density Wave
- Superconductivity

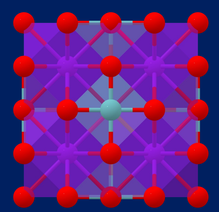
Strongly Correlated

$KTaO_3$ (Cubic)



- Optically Tunable
- Spin Transport
- Superconductivity

$KNbO_3$ (Cubic initial)



- Optically Tunable
- Phase-based Polarity
- Piezoelectricity

Goals

Goal I

- Conduct theoretical calculations for the electronic structure of $SrVO_3$ and $NbSe_2$.
- Share results with ARPES team (Dr. Brendan Faeth and Anna Capuano) to compare experimental measurements with calculations.

Goal II

- Investigate whether a non-polar material like $KTaO_3$ can become polar due to strain in the system.
- Compare with respect to $KNbO_3$, which has polar phase geometries.

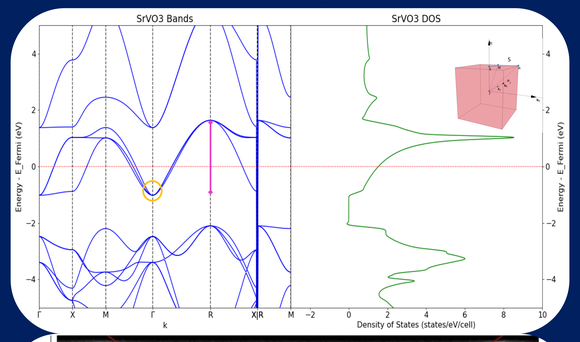
Acknowledgements

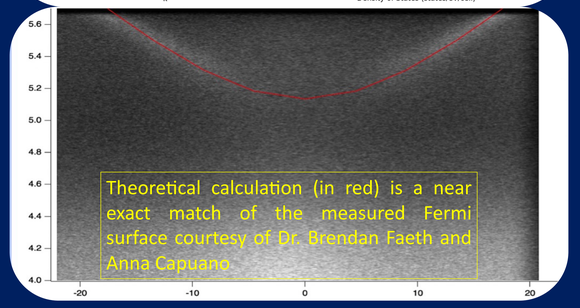
- PARADIM along with Cornell for hosting me.
- Johns Hopkins for providing the Rockfish supercluster.
- Dr. Betul Pamuk my mentor for her expert guidance and keen insight.
- Professor Darrell Schlom
- Dr. Brendan Faeth for being a wonderful collaborator.
- Jim Overhiser for being an excellent coordinator.

Results

Goal I

$SrVO_3$

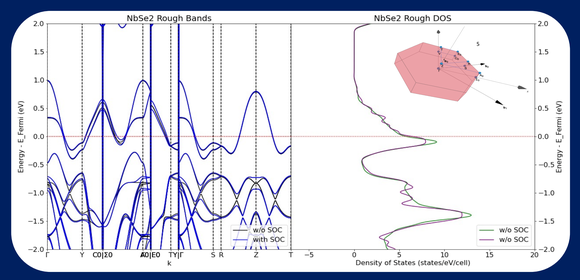




Attributes[1]

- Metal (Fermi Level through Conduction Band) ✓
- Bandwidth between 0.9 and 2.6 eV ✓
- Minima on gamma point between -1.0 and -0.4 eV ✓

$NbSe_2$

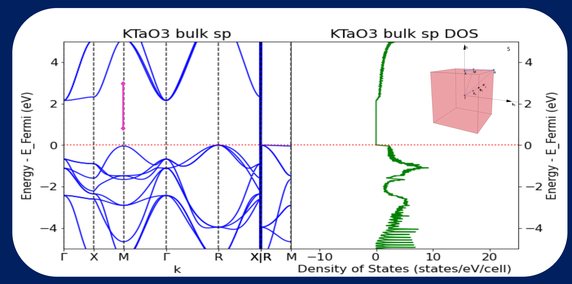


Attributes[2]

- Metal (Fermi Level through Conduction Band) ✓
- After crossing Fermi level, gap between conduction and valence from 0.35 – 0.6 eV ✓

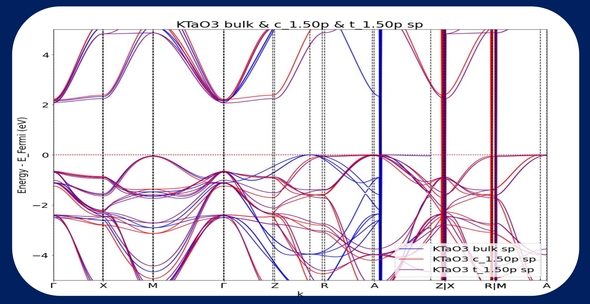
Goal II

$KTaO_3$



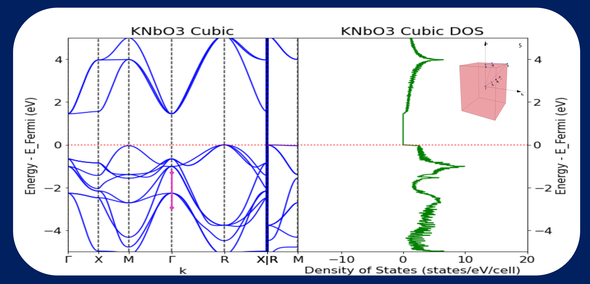
Attributes[3]

- Insulator (Fermi Level on maxima of valence band) ✓
- Gap between conduction and valence > 2 eV ✓



- The strained structures have a different and longer k-path, as the geometry has changed from cubic to tetragonal.
- Relative to bulk, the tensile strain has a lower band gap, while the compression strain has a slightly higher band gap.

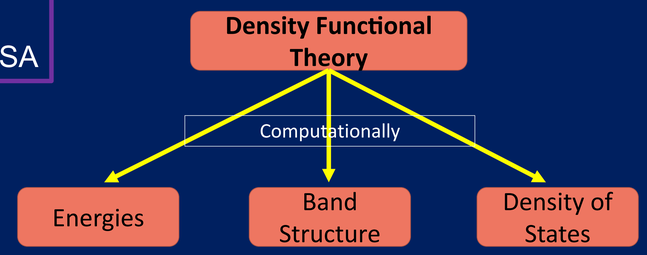
$KNbO_3$



Attributes[4]

- Similar to $KTaO_3$ except semi-conductor (gap < 2 eV). ✓

Method



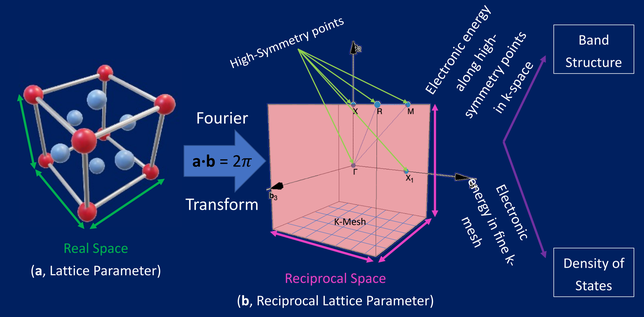
XSEDE. (2021). [Photograph]. https://portal.xsede.org/jhu-rockfish

Quantum Expresso. (n.d.). [Logo]. http://linuxtoolkit.blogspot.com/2010/05/quantum-espresso.html

- Density Functional Theory was used to calculate the electronic properties of all materials studied.
- Quantum Espresso software was used on the Rockfish cluster to conduct these calculations.
- A four-step process was used for the calculations:

Initial Self-Consistent Field → Relax / Strain → Bands → Density of States

- Band structure and Density of States can be defined as follows:



Future Work

- Optimize $NbSe_2$ structure and respective bands and density of states.
- Bands and Density of States for different $KNbO_3$ phases.
- Phonon measurements for $KTaO_3$ strains to detect instabilities.

References

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