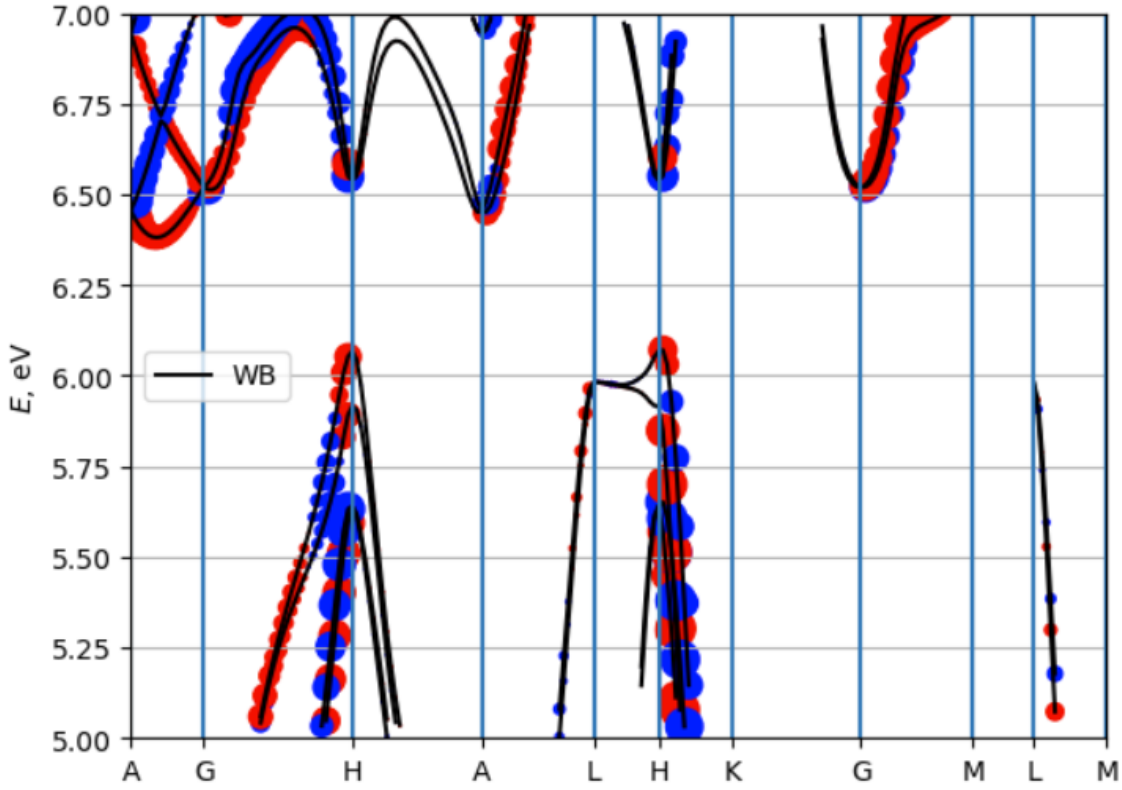
Wannier Berri Synopsis

The project code I selected is an advanced implementation of wannier functions to compute both wannier interpolation and k-space integrals.

Details

Wannier functions are orthogonal functions that play a key role in solid state physics notably within the examples and documentation of this project dealing with crystals on a molecular level. When applied to interpolate band structures (which describe the energy levels contained within the electrons of the solid structures in question) these equations can provide insights into various electronic properties of solids. This code specifically allows the user to evaluate static and dynamic quantities. These quantities are represented by a mathematical structure referred to as a Brillouin zone.



(Example of a plotted band structure from the tutorial in the notebook)

It is worth noting that in order to run the notebook, an installation of a wannierberri package is needed.

Questions

My first question is more about the concepts being applied. I would like to know more about Brillouin zones as it seems they are a collection of scattered data points to represent solid states for band structures to be identified through but the nature how it forms such an accurate representation is unclear to me.

Additionally, I am curious as to how well this project might be able to handle assessment of semi-solid state physics and or objects that are nearly solid but with some fluid dynamic elements.

Project Proposal

With this project, I would love to use the existing code to dive into some of the specifics of analysis in how it relates to some of the class topics. Perhaps creating an assessment code that plots the evaluation of the error vs cost of the wannier berri interpolation when used on a simulated dataset with known values.