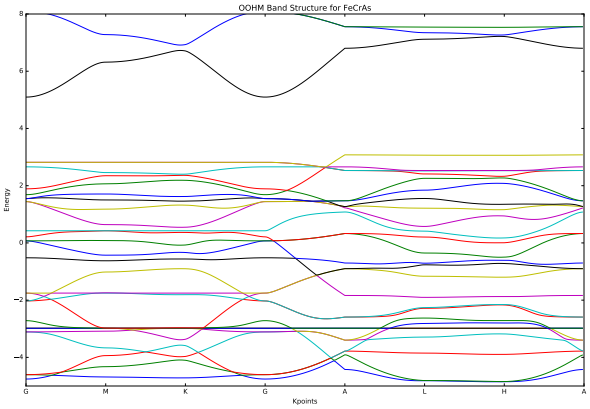

Figure 1: Band structure for all hopping parameters = 1

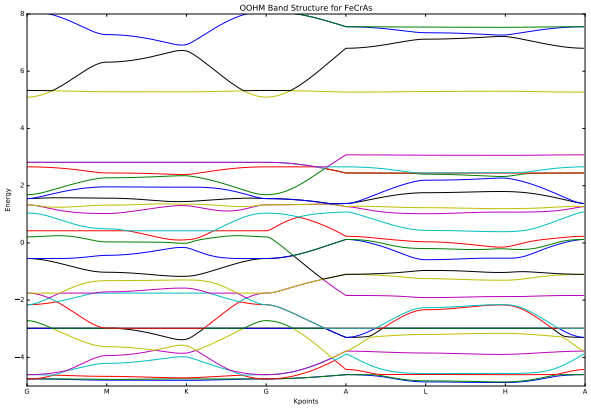

Figure 2: t-a-cr = 6

Current State

I have been engaging in a renewed fight for my first lead-author paper as a scientist. Thus far, I have reformatted my dissertation for publication in Physical Review B. In general, it looks reasonable, despite there being a need for a few adjustments. A major task that I have undertaken is the rewriting of the Optimal Overlap Hopping Model (OOHM) code in Python. There are two reasons for rewriting the OOHM code: 1) I have lost access to Mathematica because I am no longer a BU student. 2) Writing code in an open source language enables me to show my greatest coding accomplishments to prospective employers.

Band structure plots

Here I present the band structures that the code is currently giving. In early versions of my dissertation, I presented the band structure of our model with all hopping parameters set to 1, as well as with one of the hopping parameters, $t_{a,Cr}$ set to 6. With $t_{a,Cr}$ set to 6, the band structure of the OOHM had a couple of features similar to the LDA.

Observations of parameter adjustment

Some of the hopping parameters seem to have no effect on the eigenvalues of the system. The top three bands are not changed at all by changing the Fe splitting factor. They are entirely dependent on the Cr splitting.

Attempt to fit LDA

LDA band structure

Potential improvements to the code