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MSE 404: Computational MSE

A1. SCF energy calculation
*completed on prarie learn

A.2 Geometry Relaxation
*completed Prarie Learn

A3 E_{cut} Convergence

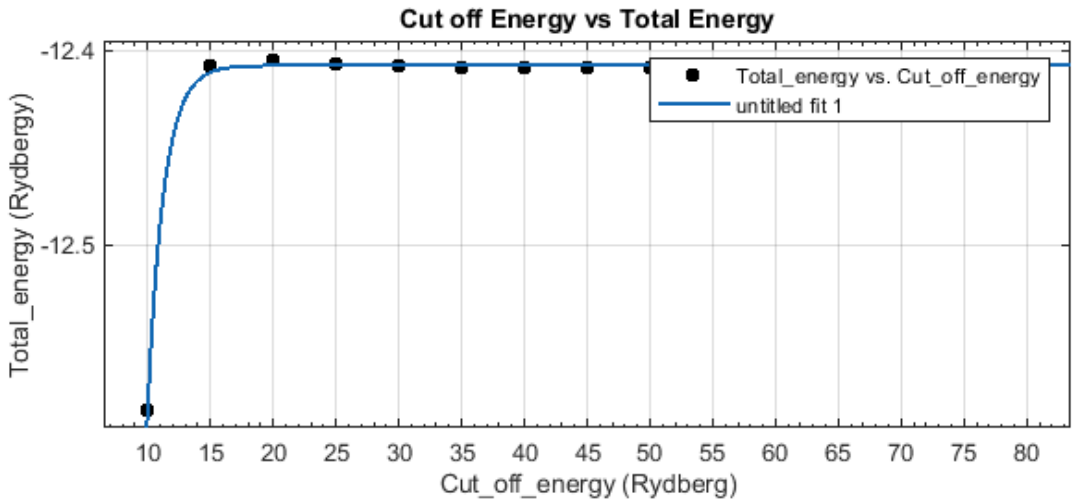

Figure 1 – Total energy with respect to Cut off Energy. This curve shows how the total energy converges over

A4. K-point convergence

***Note matlab was no longer used to plot the graphs because the fasx GUI became very slow loading and sometimes the chart properties would be hard to use**

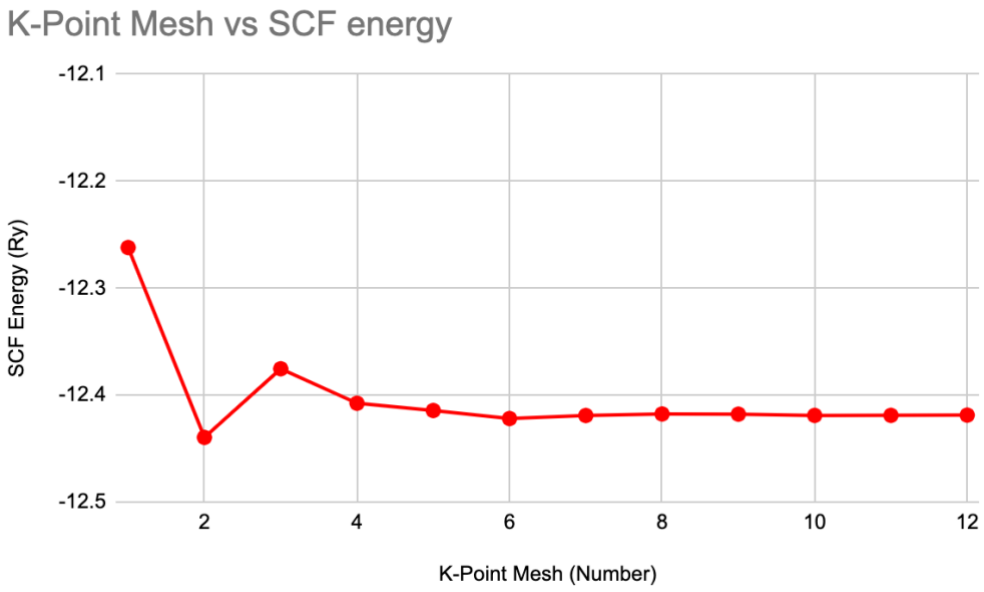

Figure 2. This figure shows how the SCF energy converges with the increase in K-point mesh.

A5. Converged Geometry

According to this source: https://periodictable.com/Properties/A/LatticeConstants.html, the lattice constant for aluminum is found to be 404.95pm. The calculated lattice constant was 7.572 Angstroms that when converted is about 396.15pm. This results in an error of approximately 2.17% error. This is a relatively small error and most of these can be attributed to the assumptions that were used under-the-hood in the QE simulation. Thus, this error is attributed to the short comings of the software simulation.

A6. Bulk Modulus

The experimentally calculated bulk modulus was found to be 848kbar. From this source: https://periodictable.com/Properties/A/BulkModulus.al.html, the bulk modulus was found to be 76 Gpa. Converting 848 kbar to Gpa, the decimal place is moved to the left one to obtain 84.8Gpa. This results in a percentage error of 11.57%. This discrepancy can be attributed to defects in the sample as in the real world not all variables can be accounted for like in a computer simulation which follows theoretical assumptions more closely.

A7. Band Structures

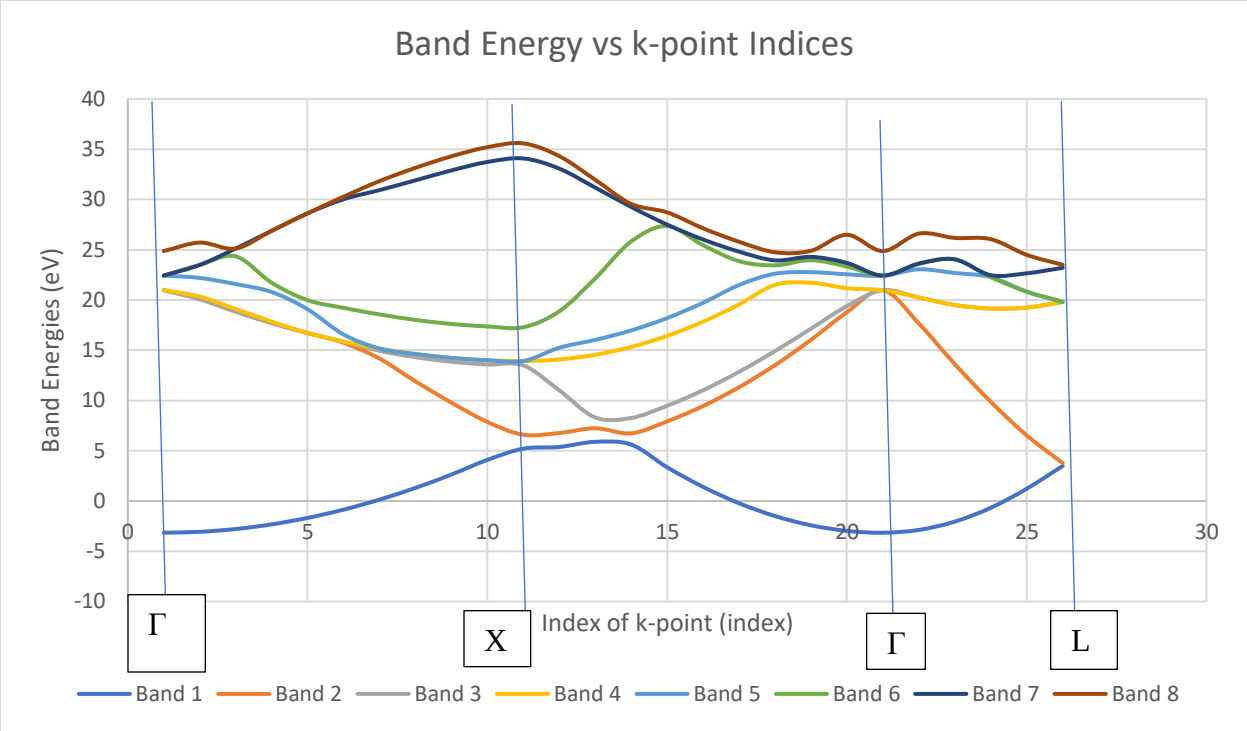

Figure 3. Acquired band structure of simulated aluminum

Neither, this is because the highest occupied orbital and the lowest unoccupied orbital come into contact at several indices of k-points. Due to this, there is not an energy band gap in which electrons can excite to. As a result, this small band gap aligns with the fact that aluminum has a small bandgap since it is a metal and allows the easy passage of electrons.