LAPW Checklist

General

- Are the number of electrons correct?
- Are the electrons distributed correctly? – filled valence bands (don't cut off any electrons at the lower energy range) – eigenvalues below ELO (check for correct positioning of energy windows)
- Is the choice of core and valence electrons appropriate?
- Check DISTANCE, Fermi energy, Total Energy as a function of iteration – are they changing smoothly and reasonably?
- Check RMS deviations ($< 10^{-3}$?)
- Check temperature variable TKB to see if it is appropriate for convergence that is desired.
- Check convergence with RKMAX.
- Correct placement of local orbitals
- Electrons lost from core?
- Compare NV with parameter NVD.

Initial

- Geometry – correct number of atoms and number of equivalent atoms – correct total number of electrons
- Make sure that core orbitals are deep and are not leaking electrons out.
- Is original core atomic configuration (as calculated with the atomic code) consistent with valence and window configuration chosen?

Output Items from LAPW code:

- GKI, GKJ, GKJ
  The code will tell you if this needs to be increase.
- If you get an error message that RKMAX was truncated, you need to increase NVD (in Comdeck P5)
- If there are no eigenvalues around 4 TKB, this implies that you have an insulator.
- If you get an error message about "ERROR IN CORED", ignore this.
  This is a problem with extrapolating the tail.
- RKMAX is invariant, independent of cell size.
- FFT grows with the linear size of the cell.
- Spin-orbit plotting: p-states only.
  $p^{1/2}$ and $p^{3/2}$ wave functions have different behavior at the origin.
  Stay away from Pb – occupied relativistic p's are a problem.
  To fix this up, would require adding local functions with the correct radial dependence of $p^{1/2}$ and $p^{3/2}$ wave functions at the origin. This would require new coding.