Running LMTO JOBS

→ *Select a compound, get the structural parameters*

→ *Run* **lminit.run** → *Produces CTRL file*

→ *Run* **lmhart.run** → *writes MT sphere radii for each species*

→ *Run* **lmovl.run** → *Check LM file for space filling*

Space filling 100 %

OK proceed

Space filling < 100 %

Run **lmes.run**

Introduces empty spheres

→ *Change verbocity to 50 and Run* **lmctl.run** → *Completes the CTRL file*

→ *Run* **lm.run** → *Check LM file for convergence*

Converged in DQ and DETOT

OK proceed

lmband.run, lmdos.run, lmfs.run

NOT converged in DQ and DETOT

Go back to iteration!