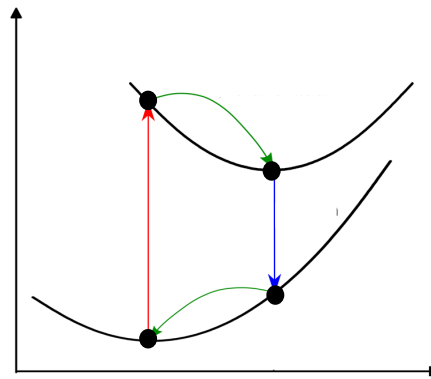


# LumiWork

- Defect supercell structure (.cif, ...)
- DFT input parameters (cut-off, tol, ...)
- Constrained occupations (... 1 1 1 0 1 0 0 ...)

- Automatized DFT tasks with  $\Delta$ SCF constrained occupation
- 2 Relaxations (ground and excited state) + 4 static scf (optional) + 4 nscf band structures (optional)
- Detection of errors, automatic restarts, ... handled by abipy



ork #0: <lumiwork, node\_id=8817, workdir=flow\_deltaSCF/w0, Finalized=true

Task	Status	Queue	MPI/Omp/Gb	Warn/Com	Class
w0_t0	Completed	4626@localhost	2  1 2.0	7  0	RelaxTask
w0_t1	Completed	4891@localhost	2  1 2.0	7  0	RelaxTask
w0_t2	Completed	4981@localhost	2  1 2.0	9  0	ScfTask
w0_t3	Completed	4989@localhost	2  1 2.0	11  0	ScfTask
w0_t4	Completed	5000@localhost	2  1 2.0	9  0	ScfTask
w0_t5	Completed	5019@localhost	2  1 2.0	11  0	ScfTask

- Abinit output files (netcdf)