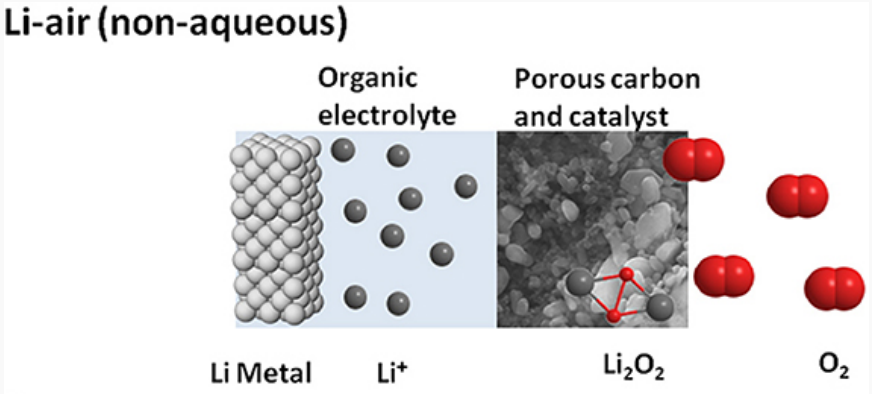
TUTORIAL SYNOPSIS

Li-air battery interface

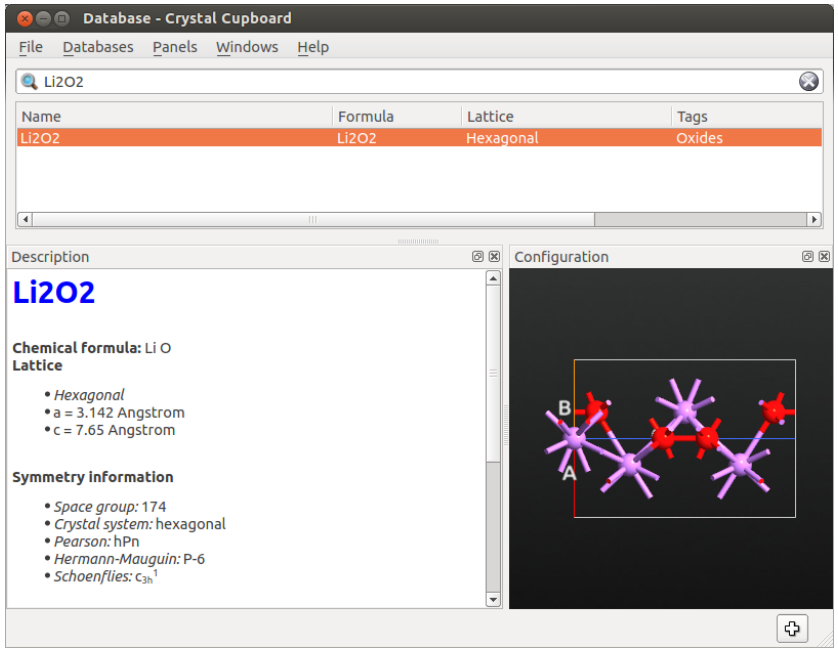
Quantum Wise
When every atom matters

- Import/create Li2O2 and Li2CO3 bulk structures
- Cleave surfaces
- Create Li2O2/Li2CO3 interface
- Create device and optimize geometry
- Calculate electronic transport properties

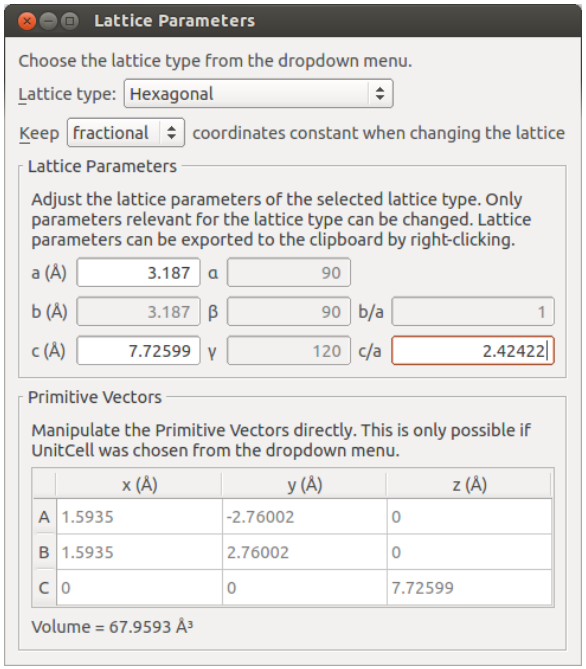


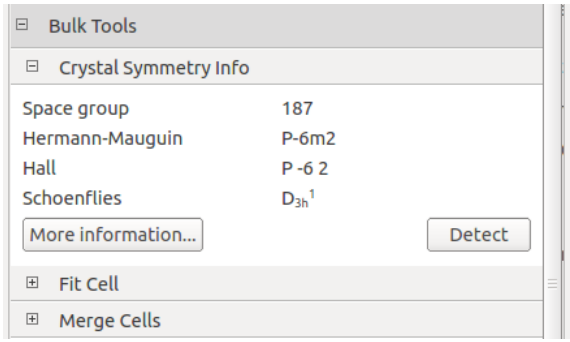
Li2O2 bulk structure

Add structure from internal database



Change lattice parameters or optimize them with DFT



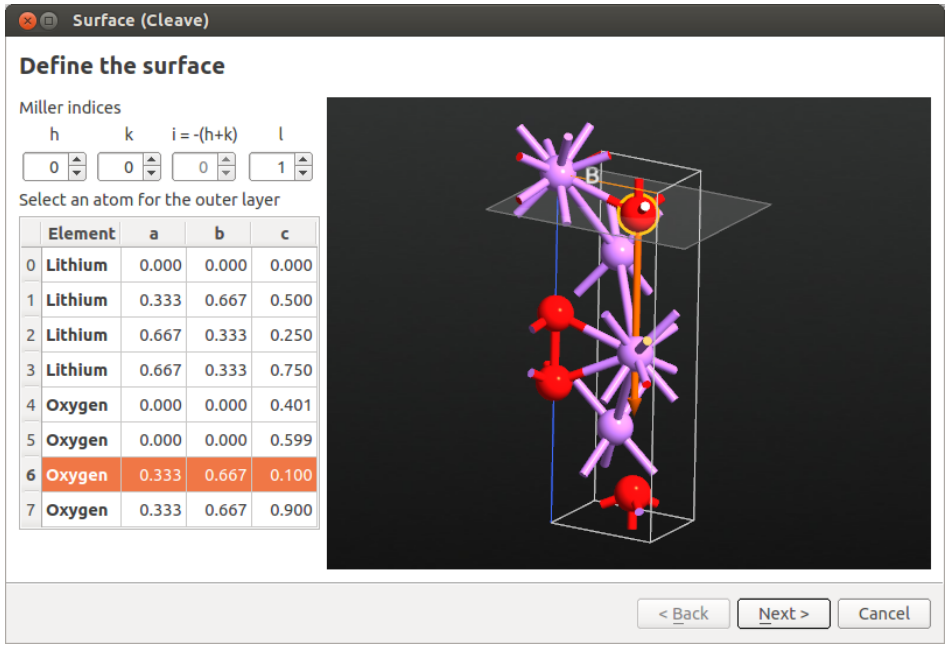


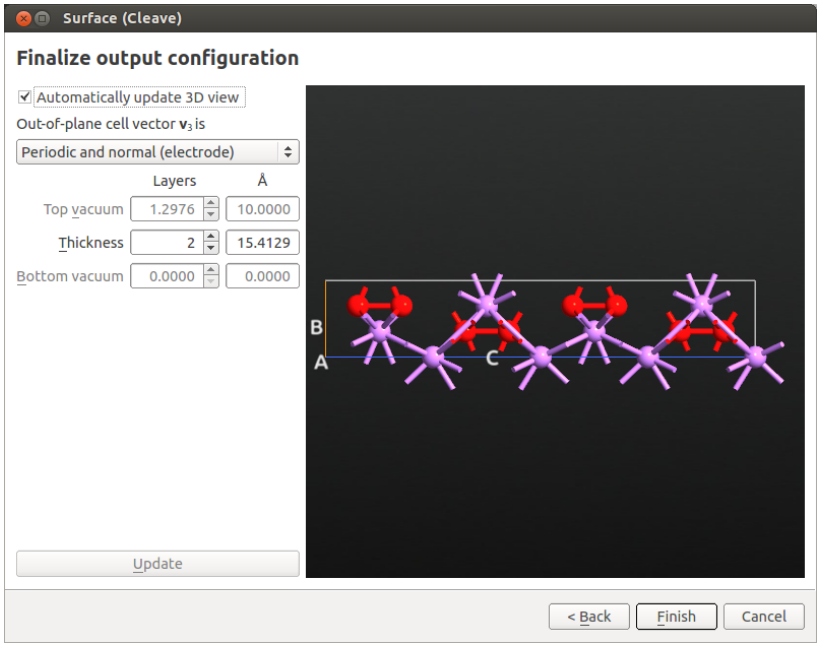
Check crystal symmetry info

Cleave Li2O2(1000) surface

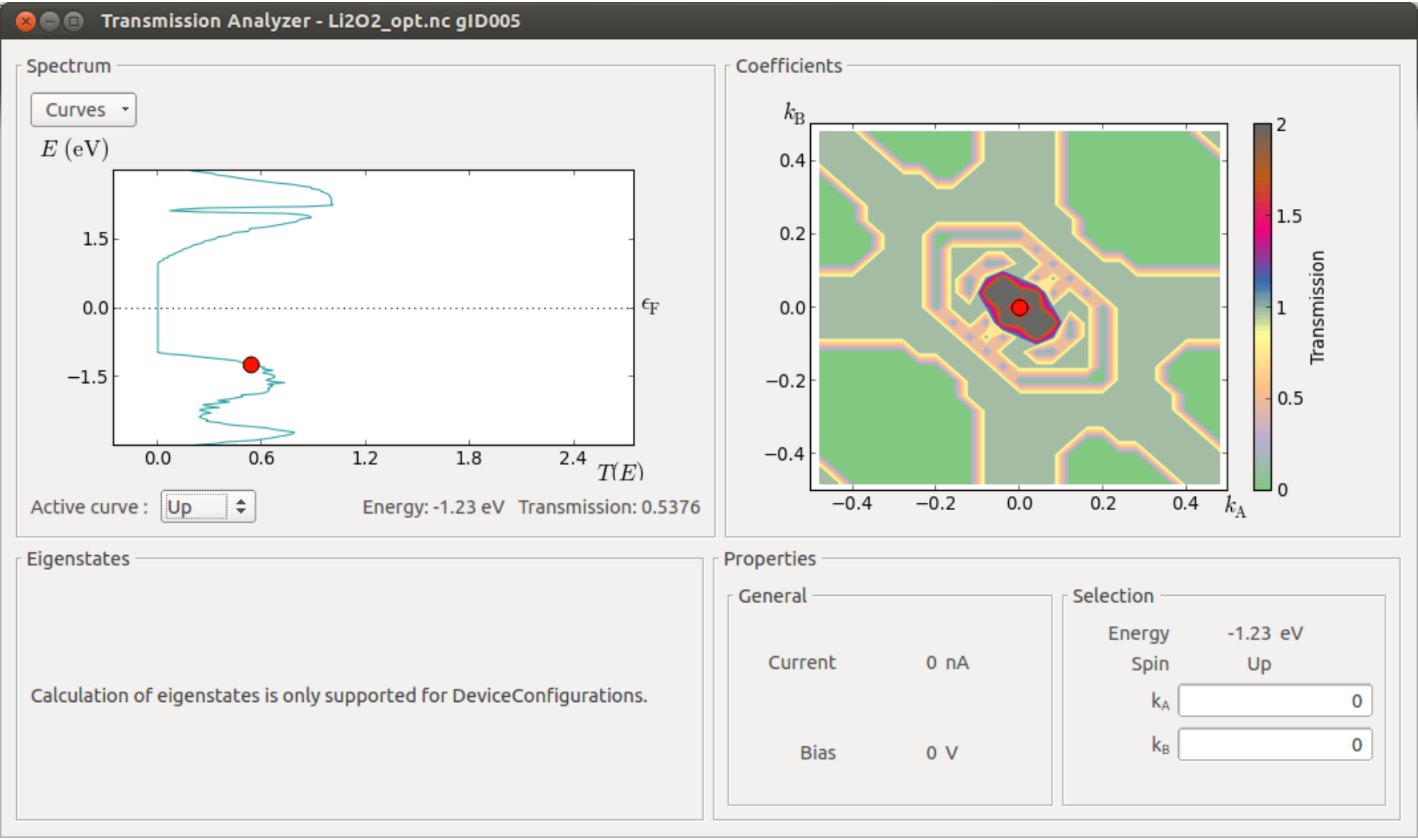
- Most stable and predominant facets (80%) in Li2O2
- during charge and discharge in nonaqueous Li-air batteries

Bulk Tools->Surface (Cleave) plugin



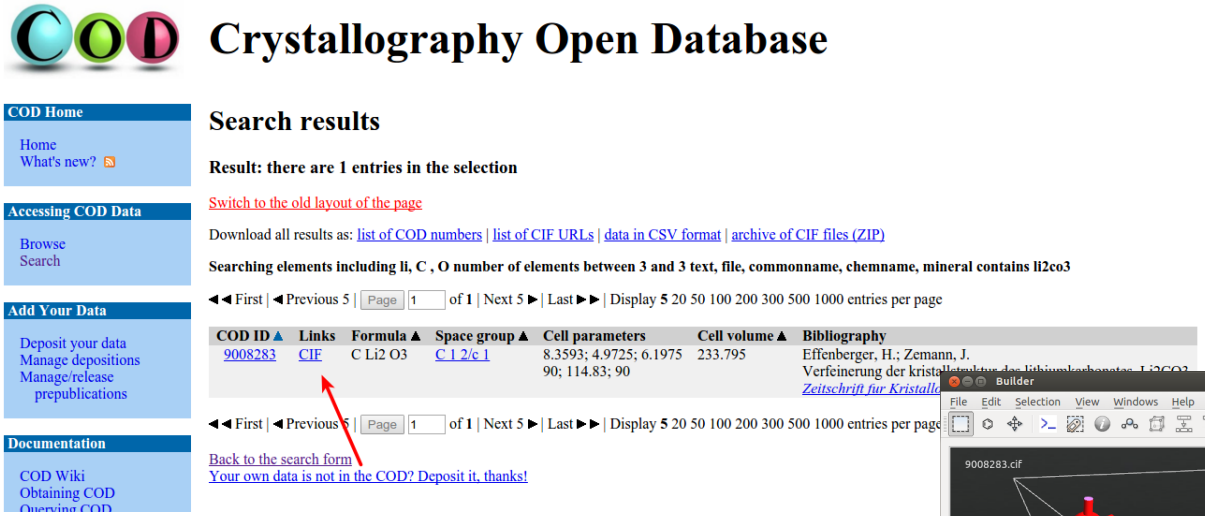


Electronic structure of Li2O2

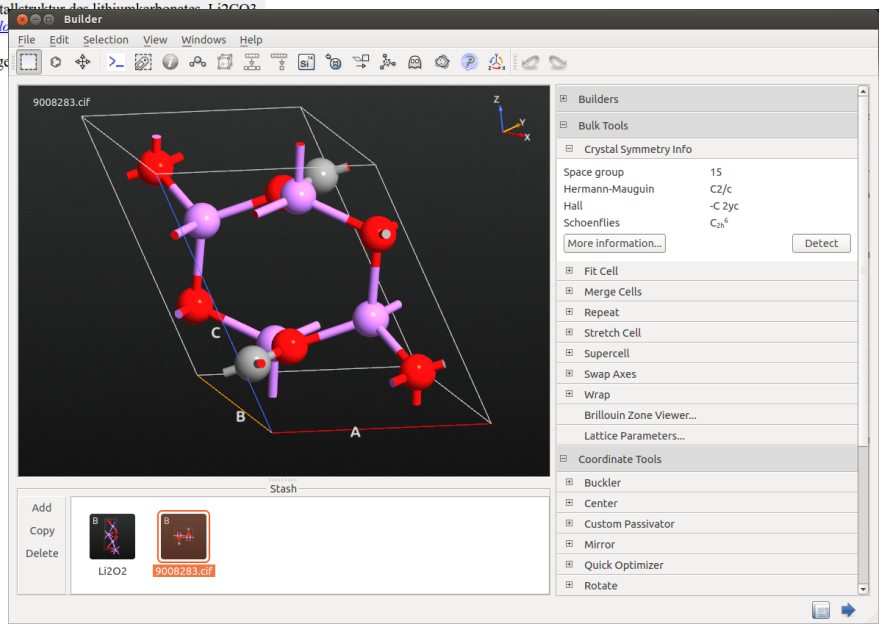


Li2CO3 bulk structure

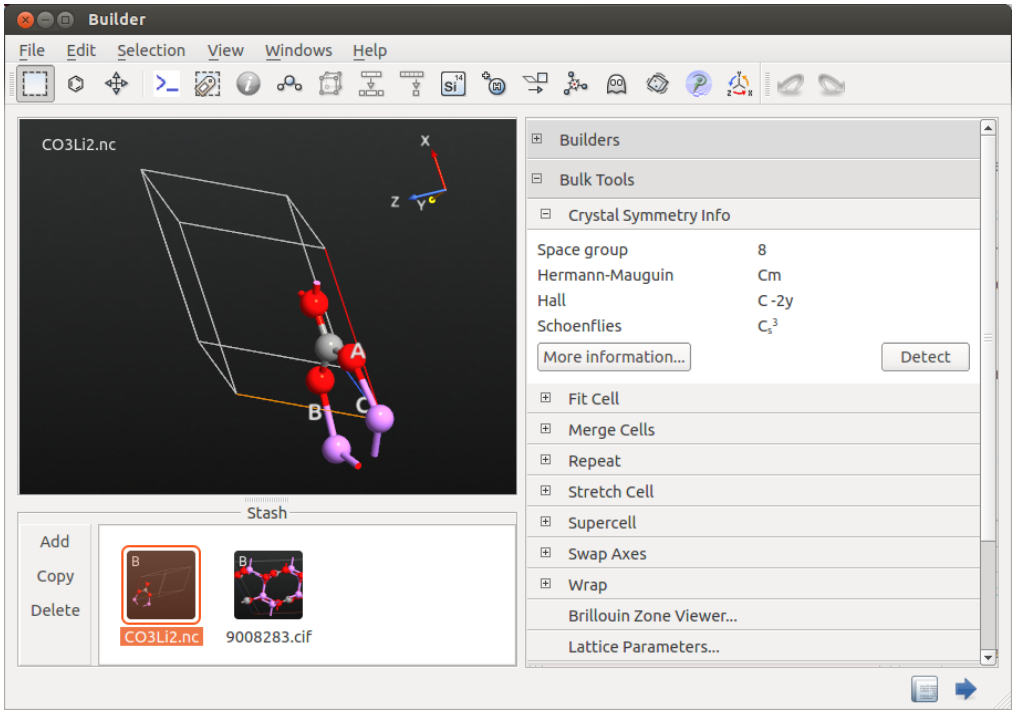
Search structure in online database, *e.g.* Crystallography Open Database, and download CIF file



Load CIF file structure in the Builder

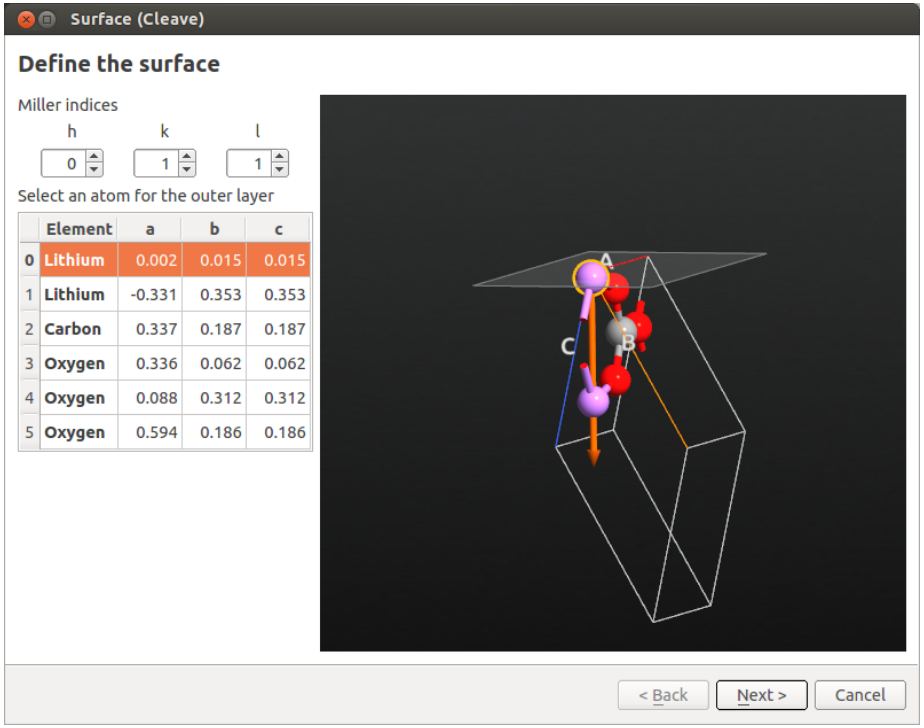


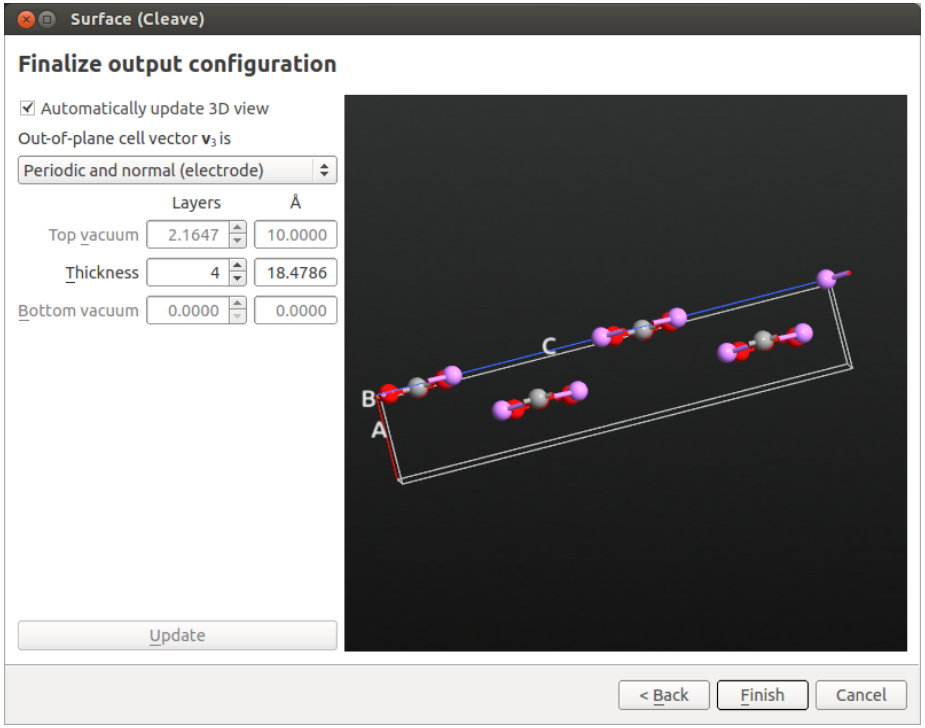
When interfacing the Li2CO3 surface with the Li2O2
you will need to use a large cell due to the lattice mismatch.
This is because the CO3 planes in the C2/c space group are slightly misaligned from the cell axes.
In this tutorial you will use a modified Li2CO3 structure with space group Cm where the CO3 planes are perpendicular to the (011) plane.
Also, this is the structure used in Yedilfana *et al.* JPCC (2015)



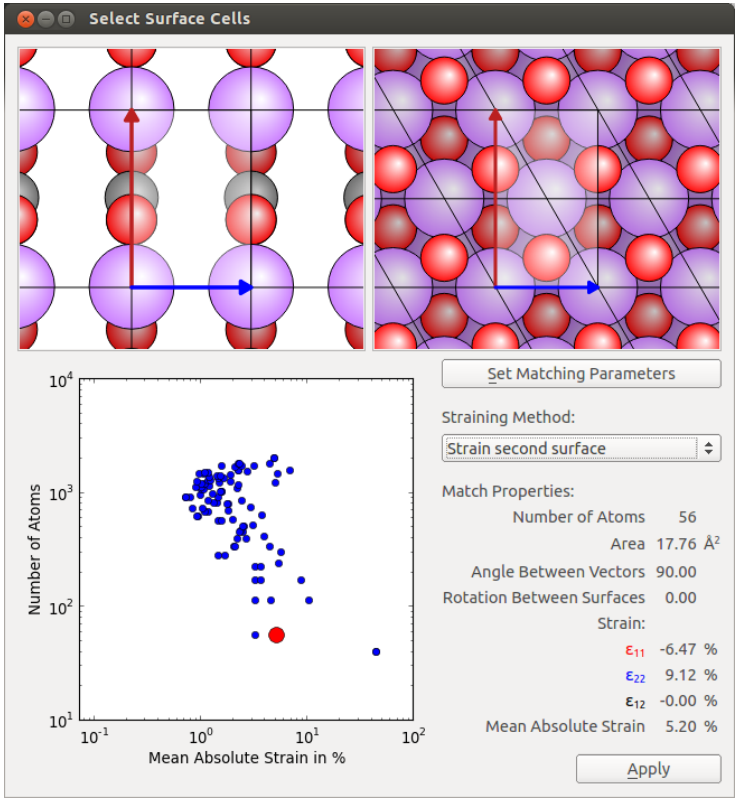
Li2CO2(011) surface

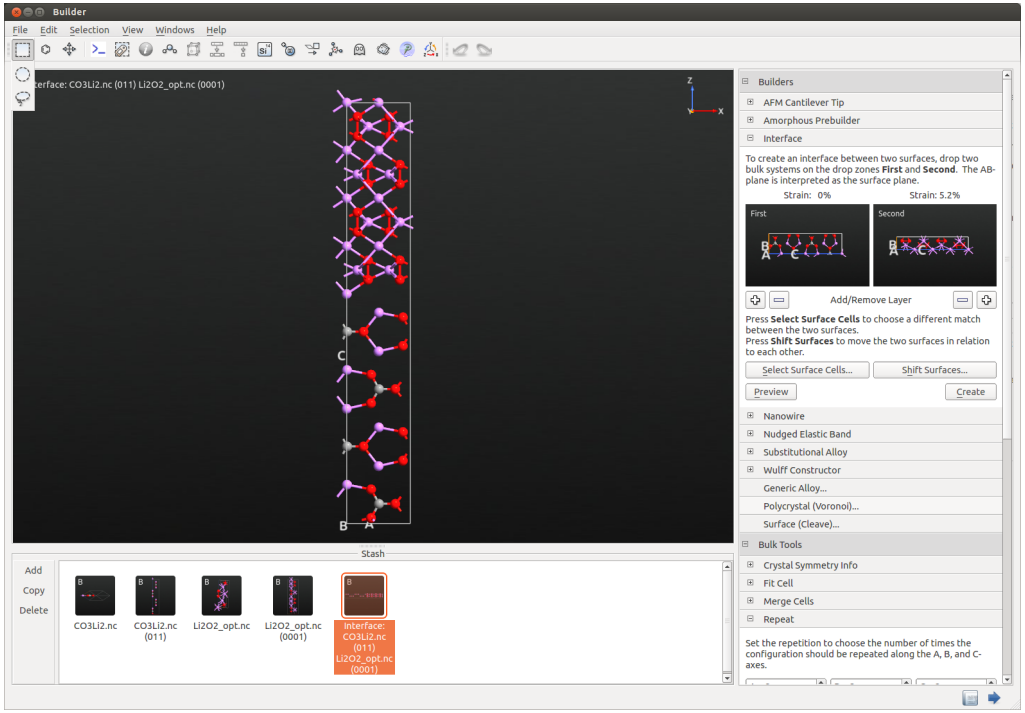
- Oxygen-terminated surface
- CO3 planes perpendicular to the CB plane





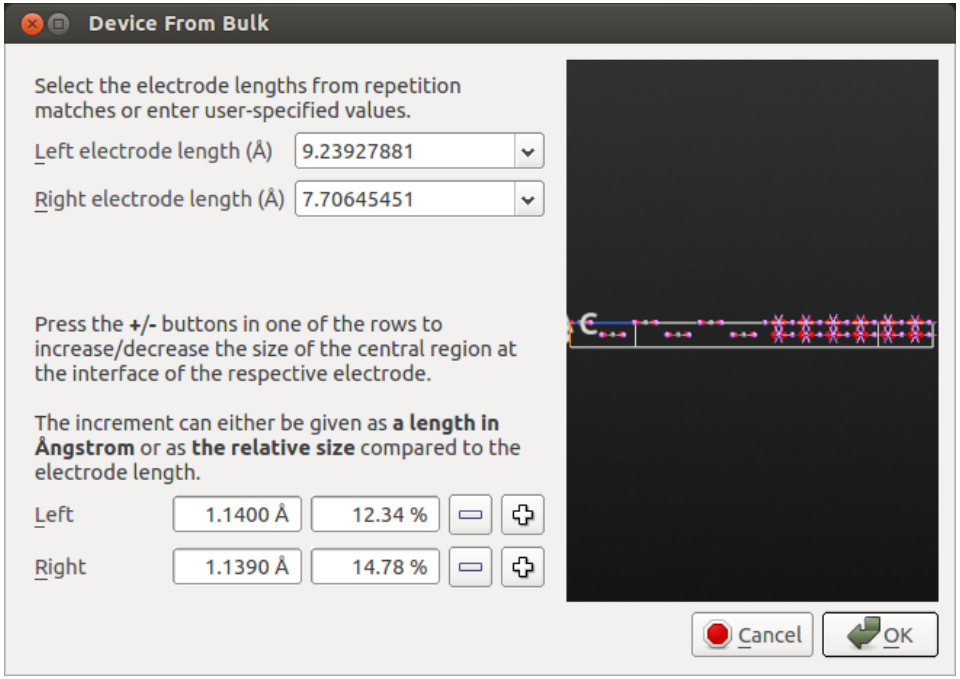
- Builders → Interface plugin
- Strain Li2O2 surface
- Mean absolute strain of 5.2%
- Depending on how you choose to cut the surface you may need to adjust the interface, *e.g.* remove Li atoms and shift surface





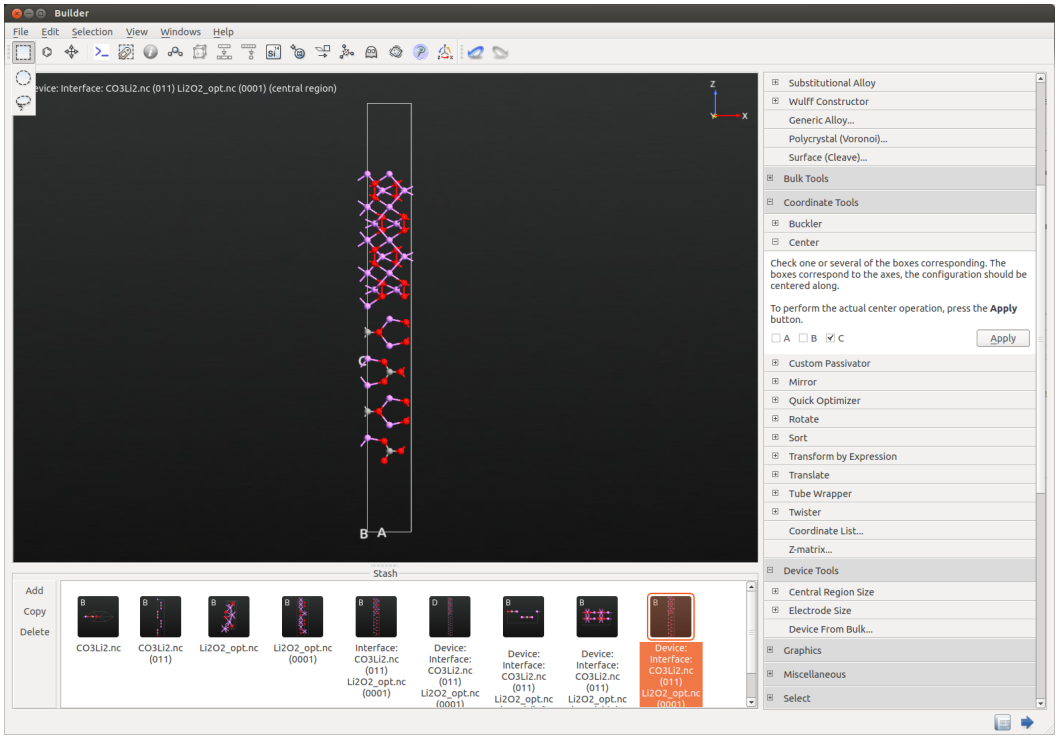
Li2CO2/Li2O2 device configuration

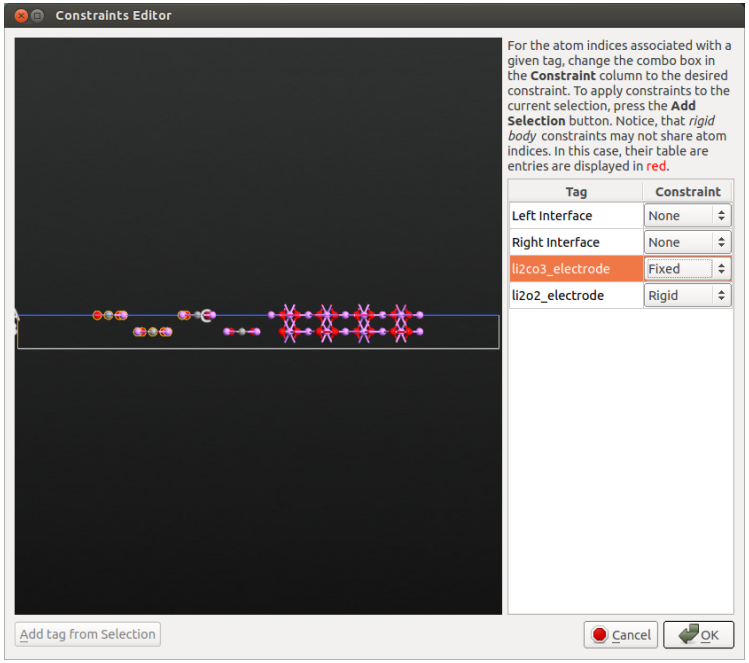
- Device Tools → Device From Bulk plugin



Li2CO2/Li2O2 geometry optimization

Optimize the interface: http://docs.quantumwise.com/tutorials/device_relaxation.html





- Take central region and add vacuum
- Tag electrode extensions + one more layer
- Optimize geometry for fixed and rigid body constrain
- Create a new device

Projected Device Density of States