GETTING STARTED WITH **DENEB** FLOWCHART

What about Bands in MgO…?

Let's calculate them using **DENEB**…

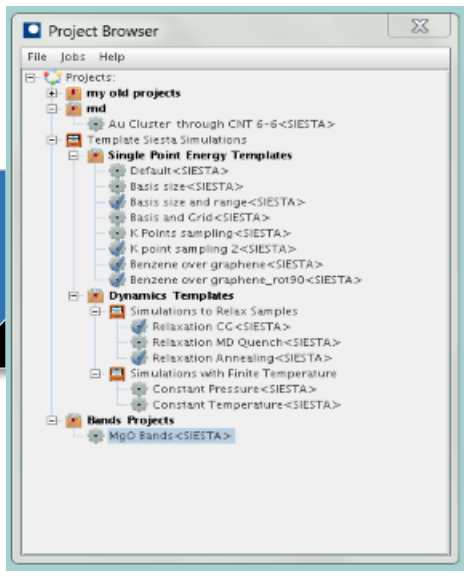
Do you have an idea?
Are you thinking about your physical system and its properties?

1

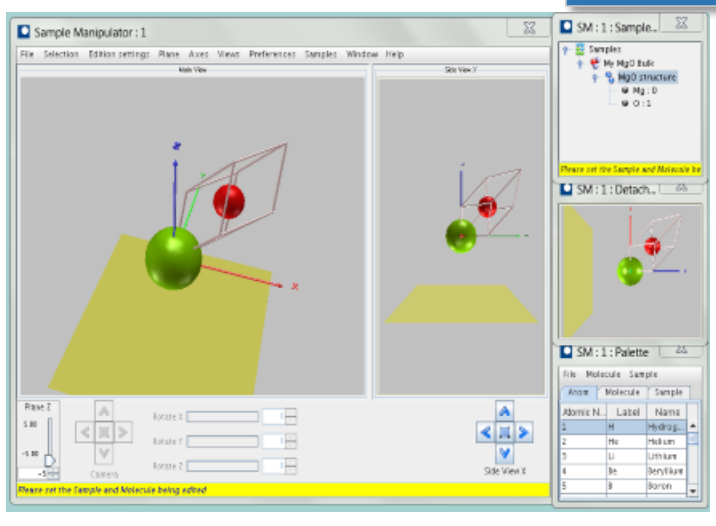
What Calculation Engine are you going to use?
Siesta for example…

2

Create in PROJECT BROWSER a new Project and a new Simulation of type Siesta



3



Do you already have your Sample of interest in NANOEXPLORER (molecule, bulk, surface, nanotube, etc.)?

NO

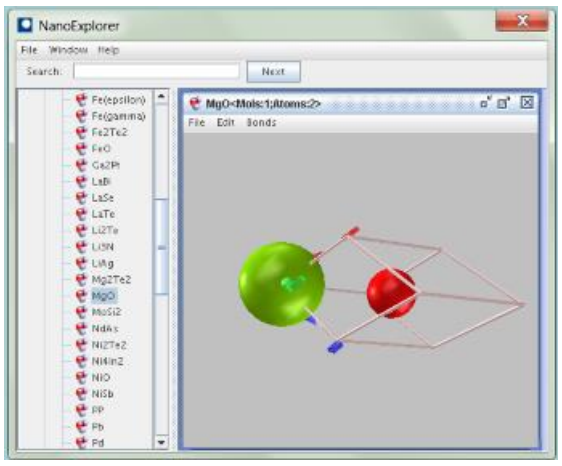
Create your Sample with a SAMPLE MANIPULATOR and store it in NANOEXPLORER to be used later

4

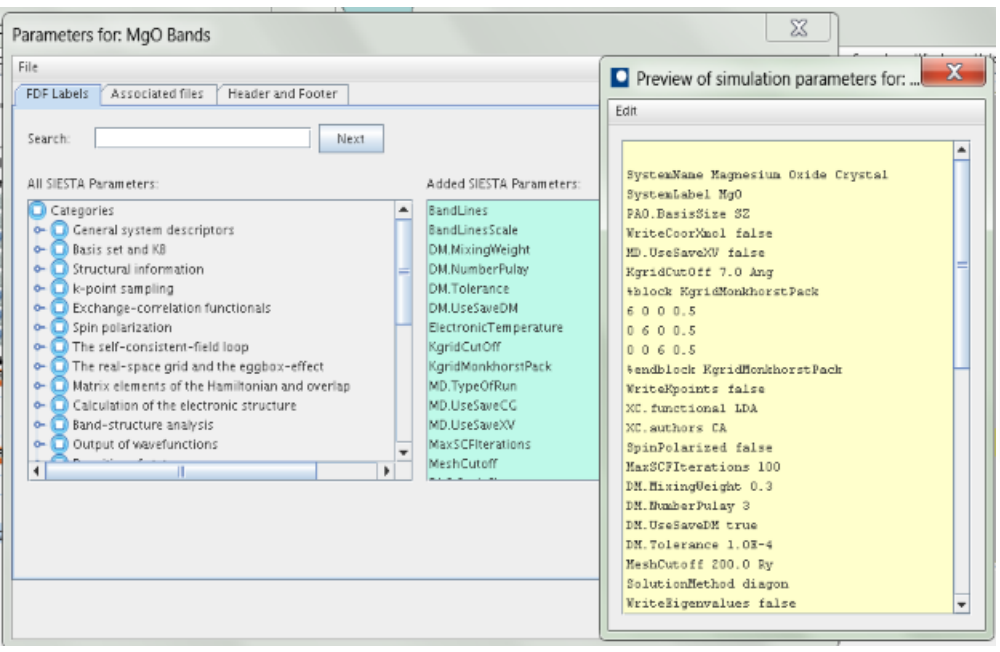
YES

Select your Sample in NANOEXPLORER and using **DENEB's** clipboard, copy and paste it into your new Simulation

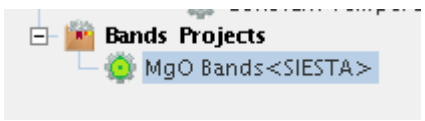
5



Set Computational Parameters and click to Run your Simulation in your machine where Siesta is installed, using one of your Engine Configurations



6



Once the remote Job has finished, **DENEB** can automatically retrieve the results for their analysis