- **Binding Energy of First Row Dimers**
- **- select a funtional (LDA or PBE)**
- **- select an element**
- **- obtain pseudopotential from the PS_libray**
- **- setup supercell for the dimer**
- **- test convegence w.r.t. cutoff (ecutwfc,ecutrho)**
- **- relax the dimer**
- **- compute binding energy and equilibrium dist.**
- **- compare with results from literature**