Gandalf

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Why Gandalf?

- `Gandalf` is a companion. This one does not perform the job in your place, but helps/accelerates considerably your job.
- This is a suite of scripts (written in python and shell) which check/evaluate the physical properties of pseudopotentials or atomic data.
- The aim is to have no boring job, human intervention, between the generation of the pseudos and an output synthesizing the main physical properties.

Example: H_2O

- You generate a pool of pseudos for Hydrogen and Oxygen (varying the pseudization radius, the number of projectors, ...) and you want to know how this affects some physical properties: atom, fcc (cohesive energy, lattice parameter, bulk modulus), dimer (binding energy, equilibrium distance)...
- What is the better compromise between the computational time (cutoff, number of projectors...) and the physical properties?
- Gandalf does not construct the input file for `Atompaw`, neither check logarithmic derivatives...
- ... but chains all these previous calculations: compute the cutoff energy "on the fly" and introduce it in the following calculations (atom, fcc, dimer), for H, O and H_2O...
- ... then concatenate all the results (table and figures) in a latex file and provide a postcript or html output.