The PseudoDojo project

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The PseudoDojo [1, 2] is an open-source python project for developing and systematically testing pseudopotentials. At present it contains four different batteries of tests executed with ABINIT and AbiPy (presence of ghost-states, delta-factor [3], GBRV benchmark [4], phonons with DFPT). The tests are performed as a function of the energy cutoff and the results are used to provide hints for the energy cutoff for actual production calculations. The pseudopotential files are available on the PseudoDojo web-interface in the ABINIT psp8 format, in the UPF2 format used by QE and in the PSML format [5] shared by SIESTA and ABINIT. The input files, the results produced by the pseudopotential generator, and the results of the tests are presented via jupyter notebooks as static HTML pages. Finally, each pseudopotential is linked to a JSON file with a full record of the different tests performed to validate the pseudopotential.

References

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