

Coding standards for the CP-PAW code

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Contents

1	Testsuite	2
1.1	Functionality tests of the main code	2
1.2	Functionality tests of tools	3
1.3	Accuracy test	3

Chapter 1

Testsuite

[1]

1.1 Functionality tests of the main code

- silicon, wave function optimization, safeortho=T
- silicon, structure dynamics (initial phonon sitortion in the structure)
- silicon, cell dynamics with fixed relative atomic positions.
- silicon, thermostats for atoms, small friction for electrons
- silicon, thermostat for atoms and wave functions
- silicon, check all options in !CONTROL!ANALYSE
- silicon, add a fraction of an electron, (charged cells)
- iron, wave function optimization, spin polarized, safeortho=F, fixed occupations
- iron, wave function optimization, spin polarized, safeortho=F, mermin block with tetra+
- iron, wave function optimization, spin polarized, safeortho=F, mermin block with mermin functional and finite temperature
- iron cell dynamics with tetra+
- NaCl, two atoms per unit cell, wave function optimization
- H₂O, wave function optimization: test isolated molecule (isolate on)
- H₂O, structure optimization: test isolated molecule (isolate on)
- OH⁻, wave function optimization: test charged isolated molecule (isolate on)
- OH⁻, structure optimization: test charged isolated molecule (isolate on)
- OH⁻: test COSMO

- Ne dimer: test van der Waals
- test !structure!orbpot
- test !structure!CONSTRAINTS

1.2 Functionality tests of tools

- silicon, band structure (Tool test)
- silicon, density of states (Tool test)

1.3 Accuracy test

- G2 database

Bibliography

- [1] P. E. Blöchl. Projector augmented-wave method. Phys. Rev. B, 50: 17953–17979, Dec 1994. doi: 10.1103/PhysRevB.50.17953. URL <http://link.aps.org/doi/10.1103/PhysRevB.50.17953>.