How to generate a mixed pseudopotential

Objectives

Generate a mixed pseudopotential to be used in the Virtual Crystal Approximation or in simulations at constant electric displacement

Most important reference

IOP PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **22** (2010) 415401 (16pp) doi:10.1088/0953-8984/22/41/415401

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How to compile the code to run the pseudopotential mixer

The code is included in the Siesta distribution, within the Util/VCA directory

Assuming we are in the directory where the Siesta sources are stored, simply

```
$ cd Util/VCA
$ make
```

It will use the same arch.make file as for the compilation of SIESTA
(no need to copy it again to the Util/VCA directory)

This will generate two executable files:

mixps (program to mix pseudopotentials)

fractional (program that multiplies the strength of a pseudopotential by a given fraction)

How to mix two pseudopotentials

Create a new directory in the directory where you generate your pseudopotentials

Copy there the two pseudos you want to mix (in this example, O and F)

```
$ cd ../atom/Tutorial/PS_Generation
$ mkdir VCA-O-F
$ cd VCA-O-F
$ cp ../O/O.tm2.psf ./O.psf
$ cd ../F/F.tm2.psf ./F.psf
```

Copy there the two pseudos you want to mix (in this example, O and F)

```
$ ~/siesta/Util/VCA/mixps O F 0.9
```

Labels of the two atoms involved

Mixing parameter: In this example
90% of the first atom
10% of the second atom

Output of the mixing of the pseudopotential

```
$ ~/siesta/Util/VCA/mixps O F 0.9
```

Labels of the two atoms involved

Mixing parameter: In this example
90% of the first atom
10% of the second atom

New files:

OF-0.90000.psf Pseudopotential file with the mixture of the two pseudos

Name of the mixed file: Symbols of the two original pseudopotentials, followed by the mixing parameter (up to five decimal places)

OF-0.90000.synth Bloch "SyntheticAtoms" to be used in SIESTA

```
%block SyntheticAtoms
 1
  2  2  3  4
    2.000000    4.100000    0.000000    0.000000
%endblock SyntheticAtoms
```

In this particular example a virtual with a charge of 6.1 electrons is generated
0.9 * 6 (electrons in O) + 0.1*7 (electrons in F) = 6,1 electrons in the Virtual Atom
2.0 electrons in the s chanel and 4.1 electrons in the p channel

MIXLABEL Final label used

Some notes on the mixed pseudopotentials

Once SIESTA reads the new mixed pseudopotential, it proceeds as usual, and generates:

- the local part of the pseudopotential
- the Kleinman-Bylander projectors
- the basis set

Those quantities are not a true mix of the corresponding quantities of the individual atoms.

The basis set is generated by SIESTA using the mixed pseudopotential (no mixing of the basis set has been implemented).

To see how to generate a basis set for a mixed atom, see the Tutorial "How to run with a finite constraint electric displacement"

Uses of the Virtual Crystal Approximation

To study substitutional disorder

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To perform calculations at constrained electric displacement
see the Tutorial “How to run with a finite constraint electric displacement”