SIESTA School 2025

Basis sets in SIESTA

Jose Angel Silva Guillén

joseangel.silva@imdea.org

Hands-on session:
Basis sets…Special cases

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EXCELENCIA SEVERO OCHOA

Exercise 1: Fixing BSSE

```
/user/path/siesta-docs/work-files/tutorials/basic/

cd basis-extra/01-WaterDimer-BSSE

ls   ->    H.psml        O.psml        dimer.fdf    monomer.fdf
           H_ghost.psml  O_ghost.psml  ghost1.fdf   ghost2.fdf
```

New files!

Created by Rihards Gromuls from Noun Project

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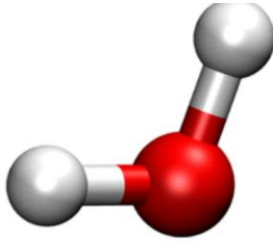
vi ghost1.fdf
```



```
%block ChemicalSpeciesLabel
 1  8  O
 2  1  H
 3 -8  O_ghost
 4 -1  H_ghost
%endblock ChemicalSpeciesLabel

AtomicCoordinatesFormat  Ang
%block AtomicCoordinatesAndAtomicSpecies
 0.000000    0.000000    0.000000 4
 0.000000    0.000000    1.522047 4
 0.436628    0.395162    0.761024 3
 2.341468    0.000000    0.760784 2
 3.795635    0.459564    0.760954 2
 3.251445   -0.331791    0.760767 1
%endblock AtomicCoordinatesAndAtomicSpecies
```

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vi ghost1.fdf
```

```
PAO.EnergyShift     0.001 Ry
%block PAO.Basis
H 1
 n=1 0 2 P 1
  0.0 0.0
O 2
 n=2 0 2
  0.0 0.0
 n=2 1 2 P 1
  0.0 0.0
H_ghost 1
 n=1 0 2 P 1
  0.0 0.0
O_ghost 2
 n=2 0 2
  0.0 0.0
 n=2 1 2 P 1
  0.0 0.0
%endblock PAO.Basis
```

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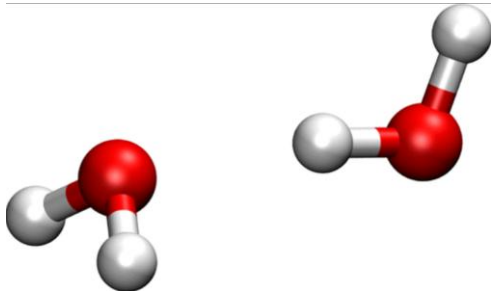
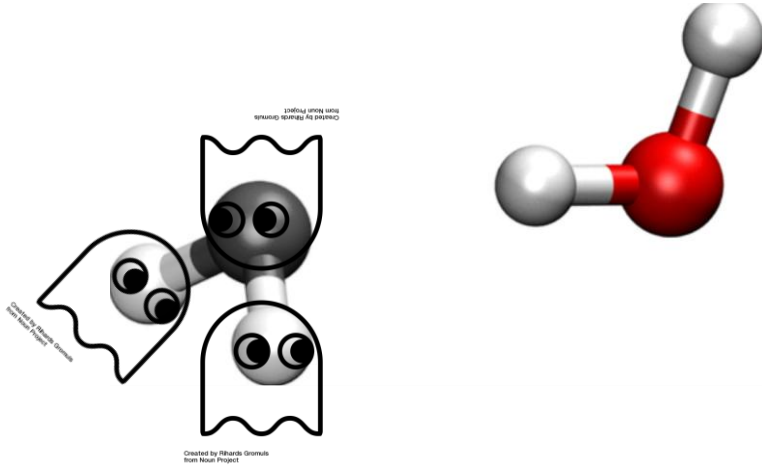
Exercise 1: Fixing BSSE

$$E_{binding} = E_{dimer} - 2 \cdot E_{monomer}$$



$$E_{binding} = E_{dimer} - E_{ghost1} - E_{ghost2}$$



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vi ghost1.fdf
```

- Excercise 1.1: Binding energy with default parameters

Exercise 1: Fixing BSSE

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           H_ghost.psml  O_ghost.psml  ghost1.fdf  ghost2.fdf

vi ghost1.fdf
```

- Excercise 1.1: Binding energy with default parameters

EnergyShift	Monomer	Dimer	Ghost1	Ghost2	No BSSE	With BSSE	BSSE	%BSSE
0.001 Ry	-482.594903	-965.509762	-482.645640	-482.646198	-320.0	-217.9	-102.1	32

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Exercise 1: Fixing BSSE

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           H_ghost.psml  O_ghost.psml  ghost1.fdf  ghost2.fdf

vi ghost1.fdf
```

- Excercise 1.1: Binding energy with Energy Shift = 0.001 Ry
- Excercise 1.2: Binding energy with Energy Shift = 0.01 Ry
- Excercise 1.3: Binding energy with Energy Shift = 0.0001 Ry

Exercise 1: Fixing BSSE

```
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ls   ->    H.psml        O.psml        dimer.fdf   monomer.fdf
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- Excercise 1.1: Binding energy with Energy Shift = 0.001Ry
- Excercise 1.2: Binding energy with Energy Shift = 0.01 Ry
- Excercise 1.3: Binding energy with Energy Shift = 0.0001 Ry

EnergyShift	Monomer	Dimer	Ghost1	Ghost2	No BSSE	With BSSE	BSSE	%BSSE
0.01 Ry	-482.136281	-964.717861	-482.174049	-482.329897	-471.9	-213.9	-258.0	55
0.001 Ry	-482.594903	-965.509762	-482.645640	-482.646198	-320.0	-217.9	-102.1	32
0.0001 Ry	-482.632604	-965.578226	-482.684753	-482.671886	-313.0	-221.5	-91.5	29

Exercise 1: Fixing BSSE

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           H_ghost.psml  O_ghost.psml  ghost1.fdf  ghost2.fdf

vi ghost1.fdf
```

- Exercise 1.1: Binding energy with Energy Shift = 0.001Ry
- Exercise 1.2: Binding energy with Energy Shift = 0.01 Ry
- Exercise 1.3: Binding energy with Energy Shift = 0.0001 Ry
- Exercise 1.4: Binding energy for the PAO.Basis block (Default parameters)
- Exercise 1.5: Binding energy for the PAO.Basis block (Rough optimization)
- Exercise 1.6: Binding energy for the PAO.Basis block (Optimized)
- Exercise 1.7: Binding energy for the PAO.Basis block (Fully optimized)

You need to add the blocks for the ghost atoms!

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Exercise 1: Fixing BSSE

```
/user/path/siesta-docs/work-files/tutorials/basic/

cd basis-extra/01-WaterDimer-BSSE
```

Results...

Basis Set	Monomer	Dimer	Ghost1	Ghost2	No BSSE	With BSSE	BSSE	%BSSE
Default	-482.136281	-964.717861	-482.174049	-482.329897	-445.3	-213.9	-231.4	51.96
Rough	-482.884135	-966.016972	-482.888456	-482.646198	-320.0	-221.9	-26.8	10.79
Opt	-482.936001	-966.119097	-247.188	-482.941834	-313.0	-228.7	-18.4	7.45
Fully opt	-482.980804	-966.205087	-966.205087	-482.986743	-243.5	-231.3	-12.2	5.02
PW J. Phys.: Condens. Matter 25, 435504 (2013)						-228.6		

Optimized basis sets -> Much better results:
- Better values
- BSSE is reduced!

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Exercise 2: Graphene

```
/user/path/siesta-docs/work-files/tutorials/basic/

cd basis-extra/02-Graphene

ls   -> C.psml  C_ghost.psml  graphene.diffuse.fdf  graphene.fdf  graphene.ghosts.fdf

vi graphene.fdf
```

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ls   -> C.psml  C_ghost.psml  graphene.diffuse.fdf  graphene.fdf  graphene.ghosts.fdf

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```

- Exercise 2.1: Change the Energy Shift 300 meV, 100 meV, 50 meV and 10 meV.
  Check the BasisEnthalpy and the TotalEnergy of the system

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vi graphene.fdf
```

- Exercise 2.1: Change the Energy Shift 300 meV, 100 meV, 50 meV and 10 meV.
  Check the BasisEnthalpy and the TotalEnergy of the system

Eshift	BasisEnthalpy	TotalEnergy
10 meV	-325.843477 eV	-326.027291 eV
50 meV	-325.992000 eV	-326.102045 eV
100 meV	-326.025687 eV	-326.111045 eV
300 meV	-325.912154 eV	-325.965841 eV

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- Exercise 2.1: Change the Energy Shift 300 meV, 100 meV, 50 meV and 10 meV.
  Check the BasisEnthalpy and the TotalEnergy of the system
- Exercise 2.2: Plot the band structure of graphene with 100 meV Energy Shift

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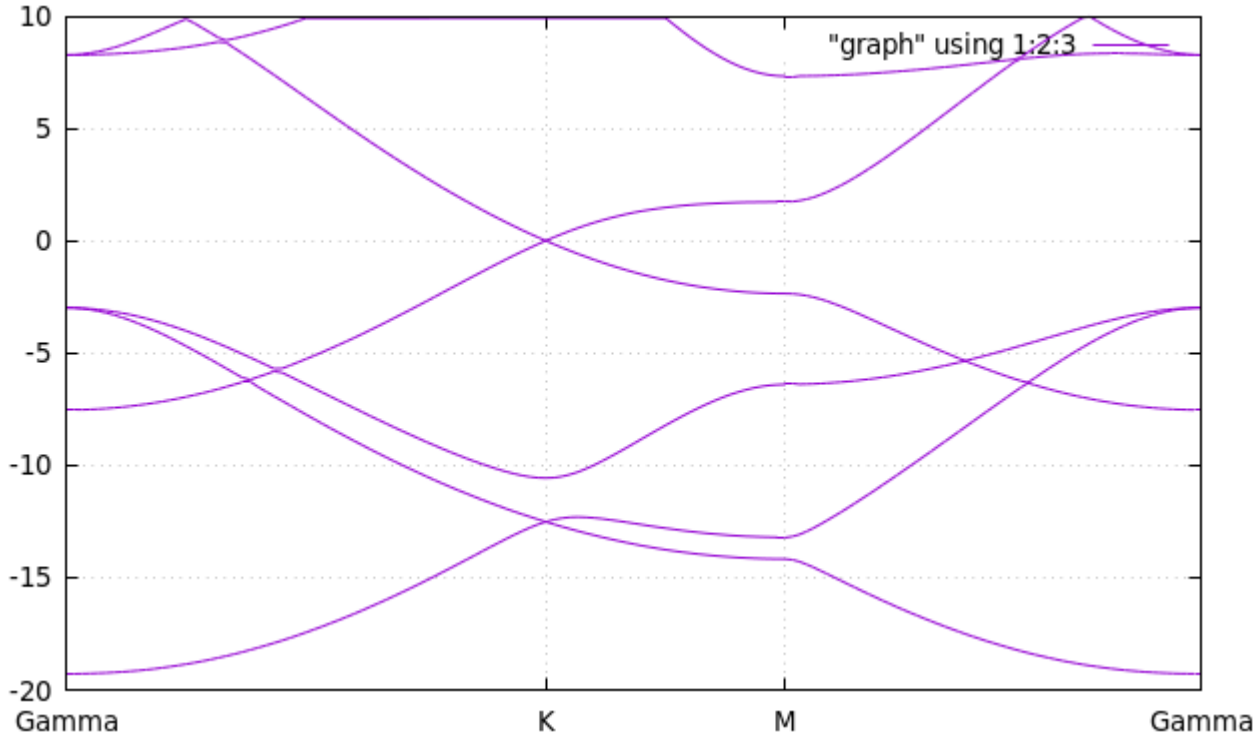
Exercise 2: Graphene



- Exercise 2.2: Plot the band structure of graphene with 100 meV Energy Shift

```
gnubands -G -F -o graph -E 10 -e -20 graphene.bands
gnuplot --persist -e "set grid" graph.gplot
```

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  Check the BasisEnthalpy and the TotalEnergy of the system
- Exercise 2.2: Plot the band structure of graphene with 100 meV Energy Shift
- Exercise 2.3: Do the same but with graphene.diffuse.fdf

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Exercise 2: Graphene

```
PAO.EnergyShift      100.0 meV
%block PAO.Basis
C        4            # We include 4 shells
 n=2   0   2          # 2s (double zeta)
   0.000      0.000
   1.000      1.000
 n=2   1   2 P   1    # 2p (double zeta) + polarization (single zeta)
   0.000      0.000
   1.000      1.000
 n=3   0   1          # 3s diffuse orbital (single zeta)
  10.000
   1.000
 n=3   1   1          # 3p diffuse orbital (single zeta)
  10.000
   1.000
%endblock PAO.Basis
```

- Exercise 2.3: Do the same but with graphene.diffuse.fdf
  vi graphene.diffuse.fdf

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PAO.EnergyShift      100.0 meV
%block PAO.Basis
C        4            # We include 4 shells
 n=2   0   2          # 2s (double zeta)
   0.000      0.000
   1.000      1.000
 n=2   1   2 P   1    # 2p (double zeta) + polarization (single zeta)
   0.000      0.000
   1.000      1.000
 n=3   0   1          # 3s diffuse orbital (single zeta)
  10.000
   1.000
 n=3   1   1          # 3p diffuse orbital (single zeta)
  10.000
   1.000              Both s and p orbitals because they can participate
%endblock PAO.Basis   in the σ band
```

- Exercise 2.3: Do the same but with graphene.diffuse.fdf
  vi graphene.diffuse.fdf

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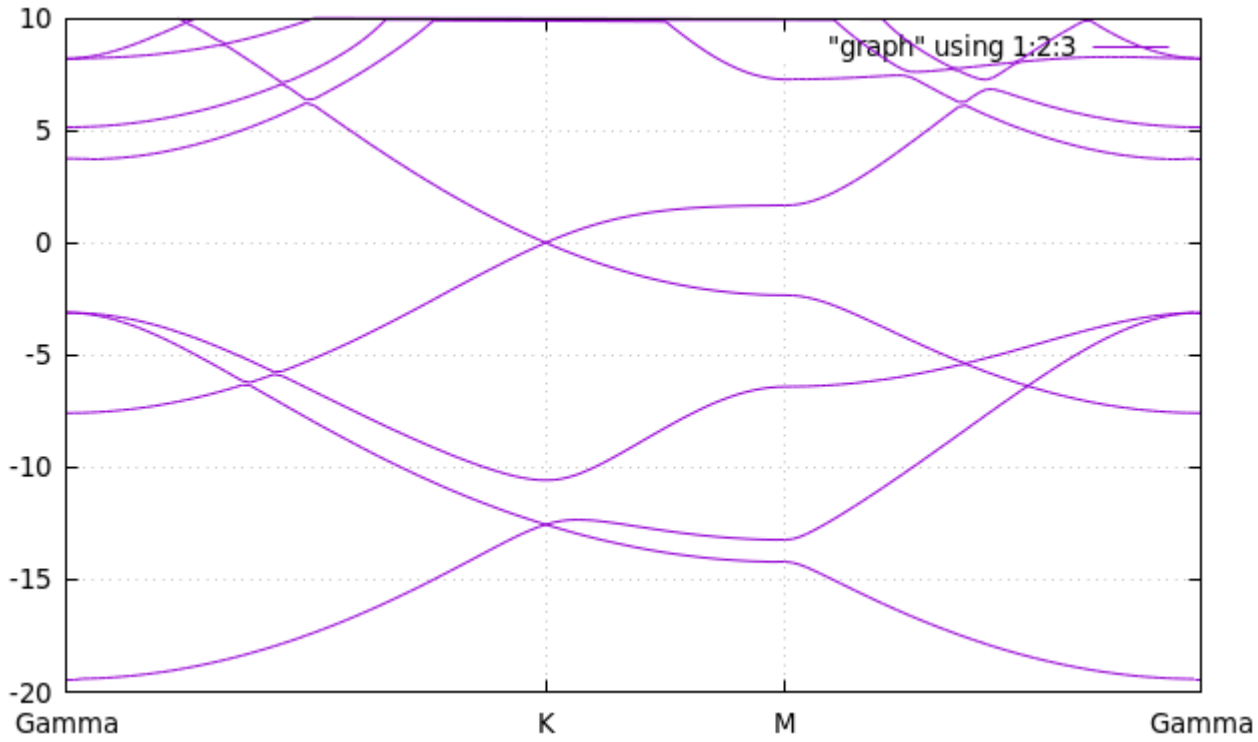

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- Exercise 2.1: Change the Energy Shift 300 meV, 100 meV, 50 meV and 10 meV. Check the BasisEnthalpy and the TotalEnergy of the system
- Exercise 2.2: Plot the band structure of graphene with 100 meV Energy Shift
- Exercise 2.3: Do the same but with graphene.diffuse.fdf
- Exercise 2.4: Play a little bit with the diffuse orbital cut-off radii.

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- Exercise 2.5: Plot the band structure with ghost orbitals (graphene.ghosts.fdf)

Exercise 2: Graphene

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- Exercise 2.4: Play a little bit with the diffuse orbital cut-off radii.
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- Exercise 2.6: Compare the results!!!

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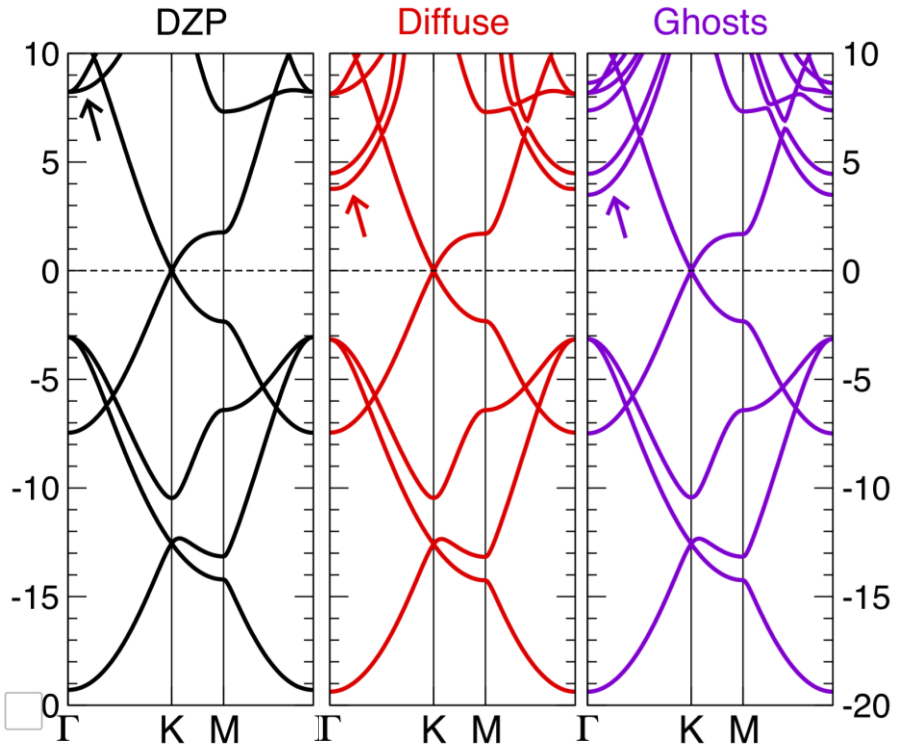

- Exercise 2.6: Compare the results!!!

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