Take-home postcard

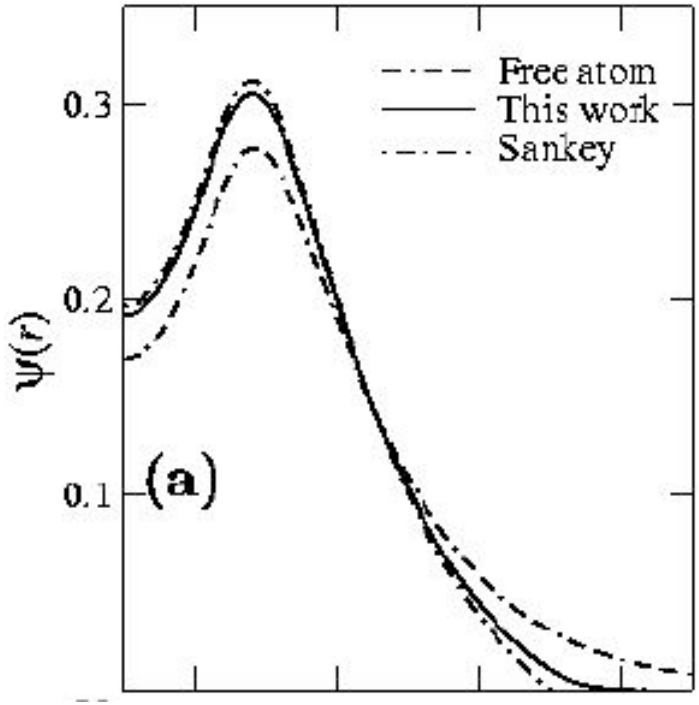
Basis set: Atomic orbitals

s

p

d

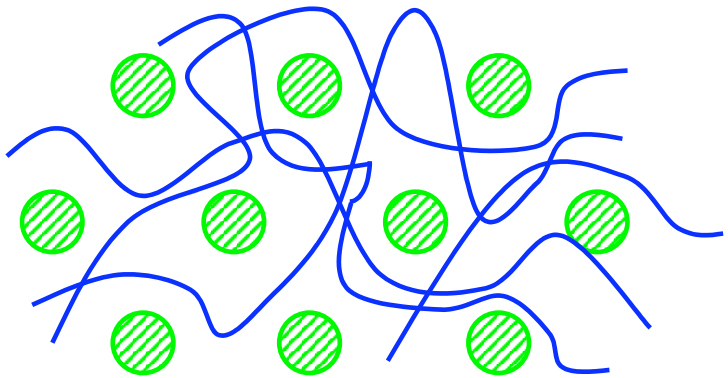
f

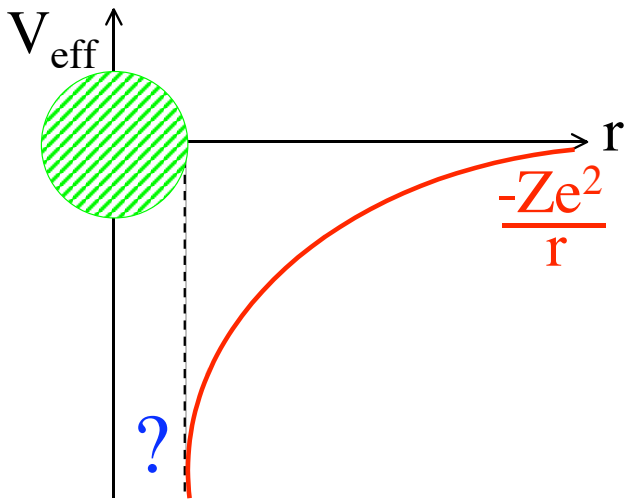


SIESTA: Strictly localized

(zero beyond cut-off radius)

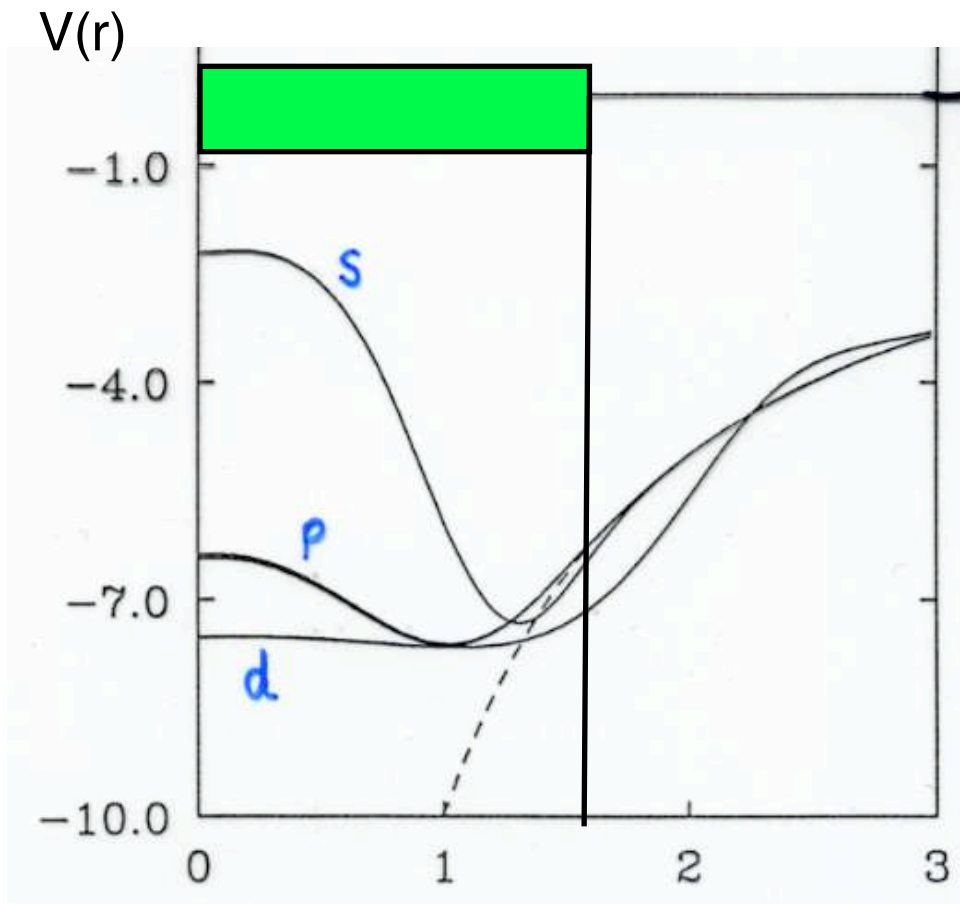
The internal electrons do not participate in the chemical bond





Effective potential for valence electrons

Pseudopotential

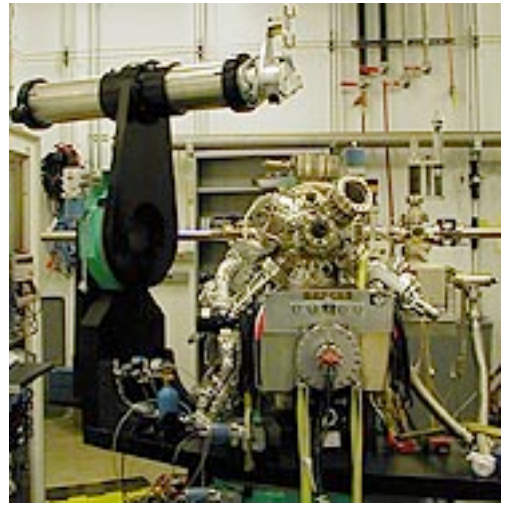


Simple taxonomy of Ab-initio codes

All electron	Pseudopotential
Muffin-Tin LAPW	Plane waves Localized Orbitals

Things to keep in mind

- Pseudopotential generation
- Number of k-points
- Electronic temperature
- XC functional: LDA, GGAs
- Harris functional vs SCF
- Spin polarization
- SCF convergence tolerance
- Supercell size (solid & vacuum)
- Geometry relaxation tolerance



Lab Apparatus

Plane-wave cutoff

PW codes

- Basis set:
  - Size (SZ, DZ, DZP...)
  - Range
  - (Shape)
- Real space mesh cutoff

SIESTA

Basis Size

Depending on the required accuracy and

available computational power

Quick and dirty calculations

Highly converged calculations

Minimal basis set

(single- ζ; SZ)

Complete multiple-ζ

+

Polarization

+

Diffuse orbitals

+ Basis Optimization

Easy setup with reasonable defaults

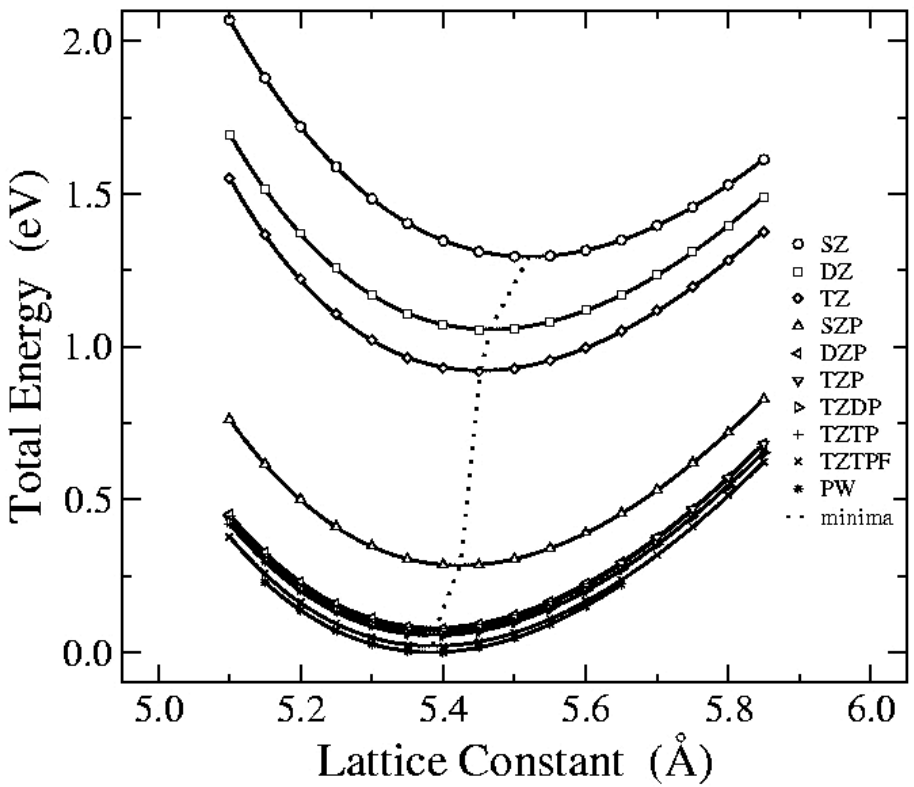
```
NumberOfSpecies         1
number-of-atoms         2

LatticeConstant     5.43 Ang
%block LatticeVectors
  0.0  0.5  0.5
  0.5  0.0  0.5
  0.5  0.5  0.0
%endblock LatticeVectors

%block ChemicalSpeciesLabel
  1  14  Si
%endblock ChemicalSpeciesLabel

AtomicCoordinatesFormat  Fractional
%block AtomicCoordinatesAndAtomicSpecies
    0.0   0.0   0.0    1  Si         1
    0.25  0.25  0.25   1  Si         2
%endblock AtomicCoordinatesAndAtomicSpecies
```

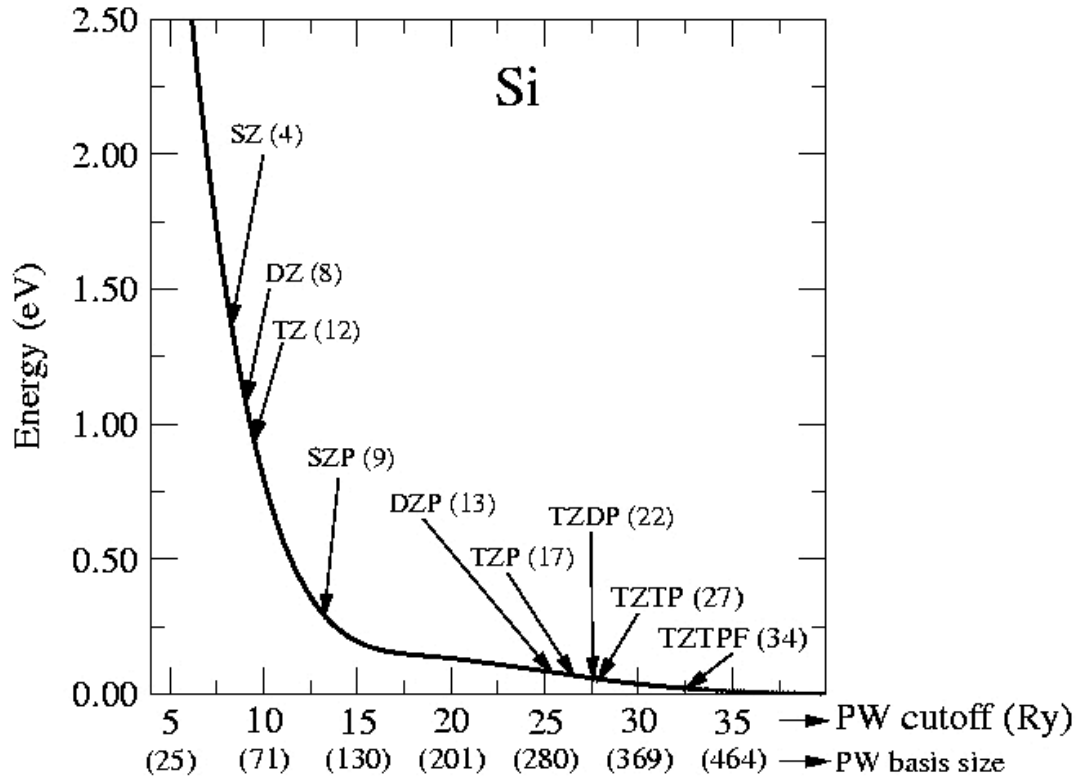
Simple level of specification

```
PAO.Basis.Size  SZP          SIZE
PAO.EnergyShift 150 meV      RANGE
PAO.SplitNorm  0.25          SHAPE


#--------------------------

MeshCutoff  200 Ry
```

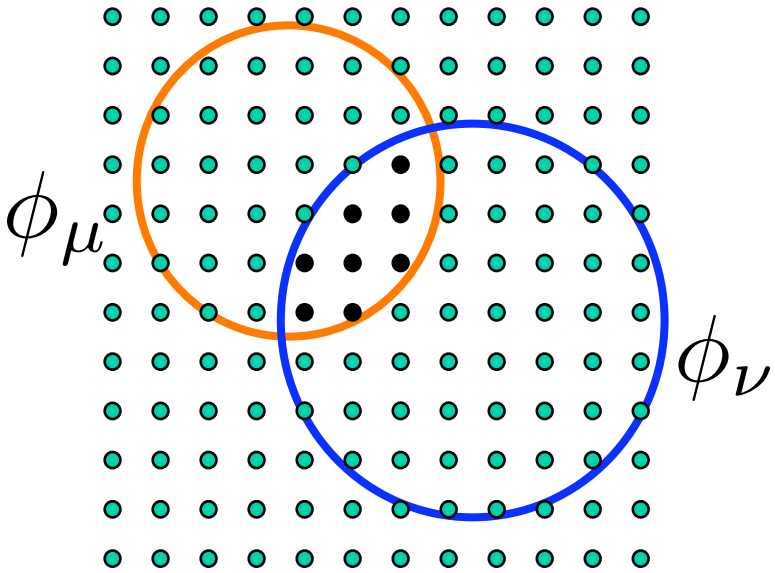
Higher degree of control

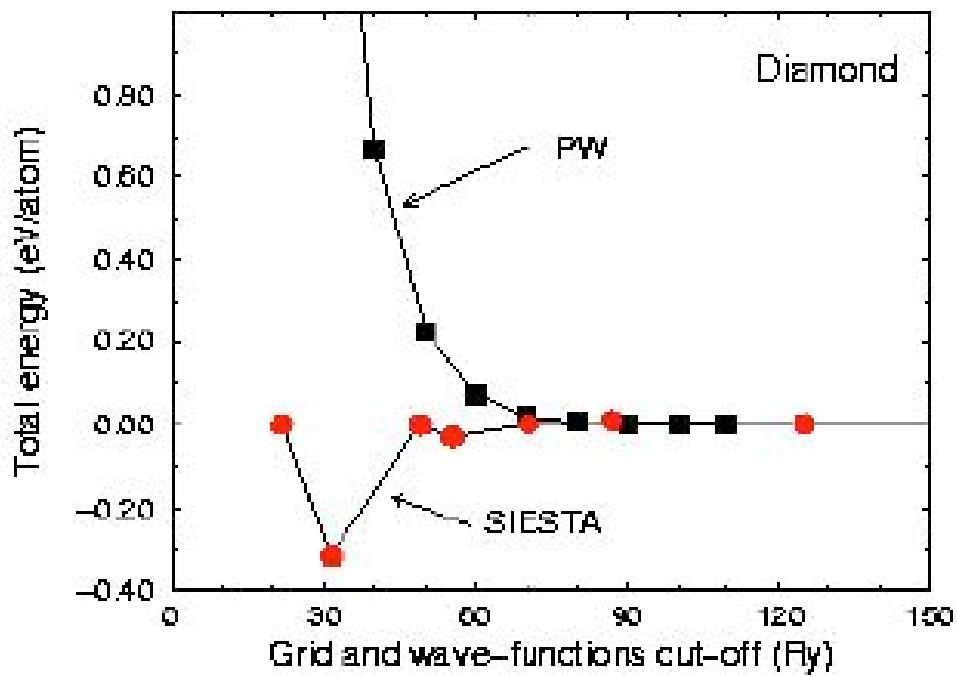
```
%block PAO.Basis
H  2      0.5
n=1 0 2
 3.5 2.8    E 40.0 3.0
 1    1
n=2 1 1
 4.5
 1
%endblock PAO.Basis
#----------------------

Grid.Cell.Sampling T
```

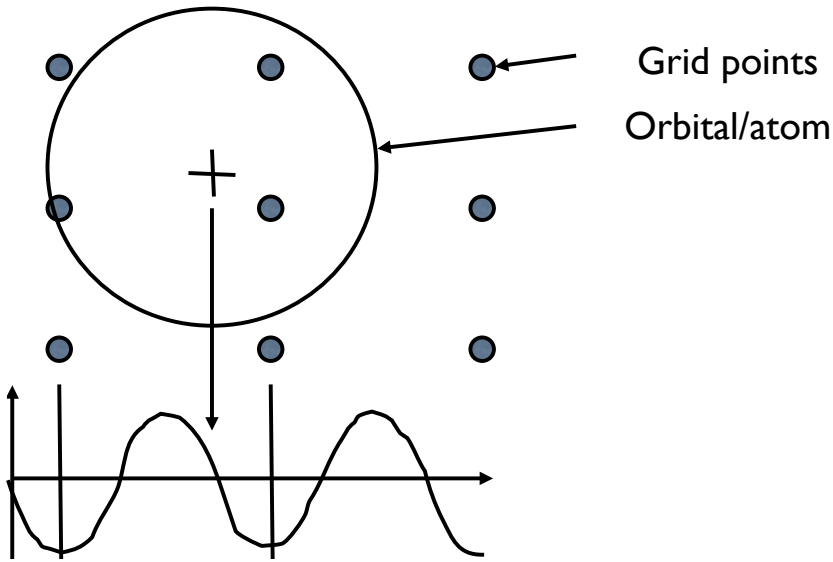

Total Energy (eV)
Lattice Constant (Å)
2.0
1.5
1.0
0.5
0.0
5.0
5.2
5.4
5.6
5.8
6.0
SZ
DZ
TZ
SZP
DZP
TZP
TZDP
TZTP
TZTPF
PW
minima


Si
Energy (eV)
2.50
2.00
1.50
1.00
0.50
0.00
SZ (4)
DZ (8)
TZ (12)
SZP (9)
DZP (13)
TZP (17)
TZDP (22)
TZTP (27)
TZTPF (34)
5
10
15
20
25
30
35
PW cutoff (Ry)
(25)
(71)
(130)
(201)
(280)
(369)
(464)
PW basis size

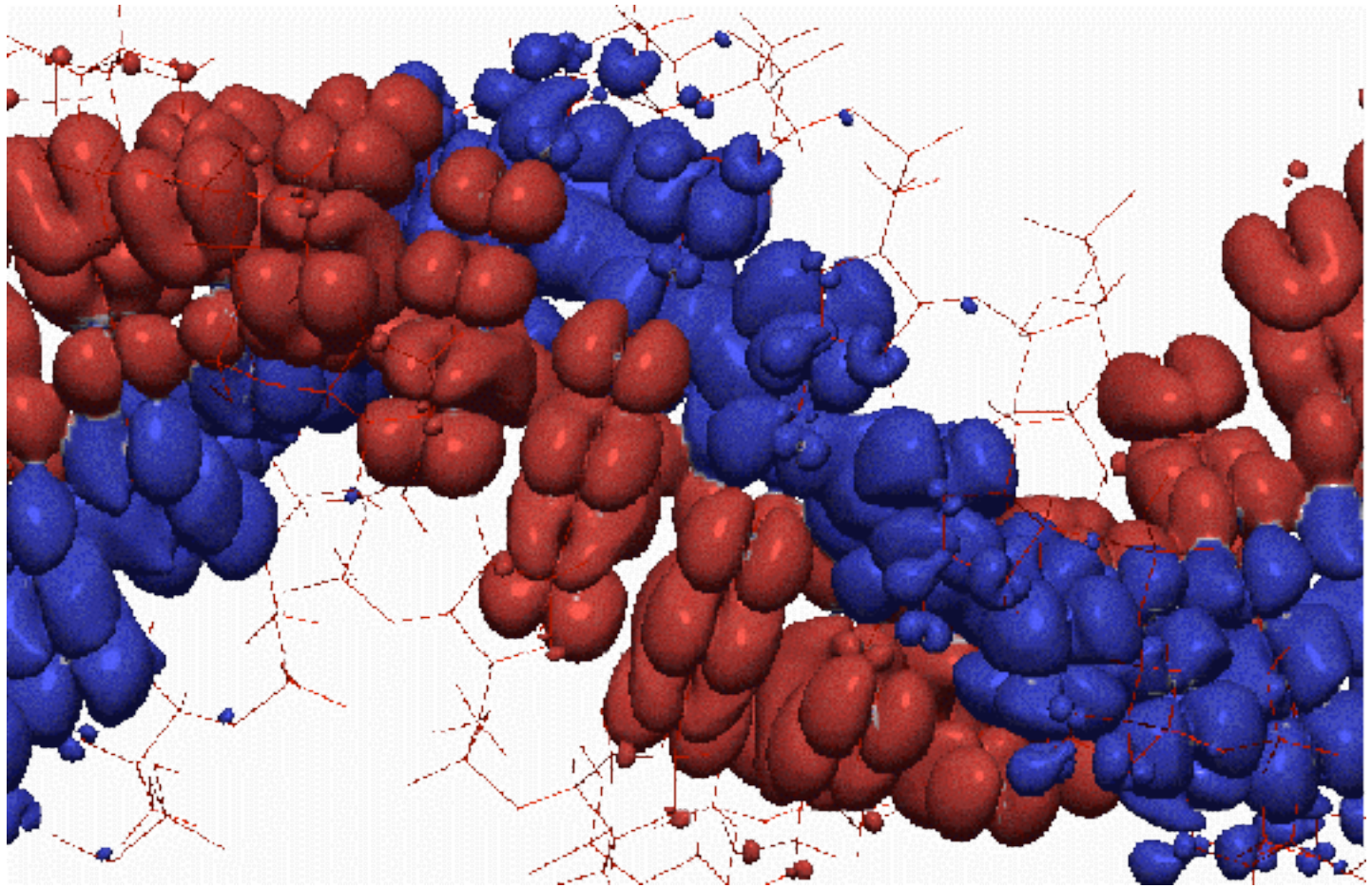
Real-Space Grid







Eggbox effect



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