

Introduction to the SIESTA code



Javier Junquera



Most important references followed in this lecture

INSTITUTE OF PHYSICS PUBLISHING

JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 2745–2779

PII: S0953-8984(02)30737-9

The SIESTA method for *ab initio* order- N materials simulation

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Javier Junquera^{1,5}, Pablo Ordejón⁶ and Daniel Sánchez-Portal⁷

SIESTA: Recent developments and applications

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30 years of SIESTA



What is SIESTA?

(<http://www.icmab.es/siesta>)



Method and its implementation in a **simulation code of atomic systems**

Solves numerically the **quantum mechanic equations**
that rule the behaviour of the **electrons**

Allows the determination of the **atom dynamics** and
simulate physical and chemical processes that
happen at the atomic scale

EVERYTHING FROM FIRST-PRINCIPLES

First-principles calculations are free of parameters but not free of approximations

Use a set of “**accepted**” approximations
to solve the corresponding equations on a computer

NO EMPIRICAL INPUT

**Quantum mechanics enables the study of materials
at the atomic level without experiments**

What are the main approximations?

Born-Oppenheimer

Decouple the movement of the electrons and the nuclei.

Treatment of electron-electron interactions.

Wavefunction theory and density functional theory (DFT)

Pseudopotentials

Treatment of the (nuclei + core) — valence.

Basis set

Restrict the electronic wave function to the space of linear combination of a finite number of basis functions

Numerical evaluation of matrix elements

Efficient and self-consistent computations of Hamiltonian and Overlap matrices.

Supercells

To deal with periodic systems

What makes SIESTA different?

Efficiency

SIESTA is a first-principles code, based on Density Functional Theory...
...as many others

Wien-2K
ELK

VASP
Abinit
Quantum Espresso
CASTEP
GPAW
Octopus

FHI-Aims
CP2K
CONQUEST
PLATO
Open-MX
DMOL
BigDFT
Quantum ATK

Gaussian
CRYSTAL
ADF
Qchem
Nwchem
Turbomol

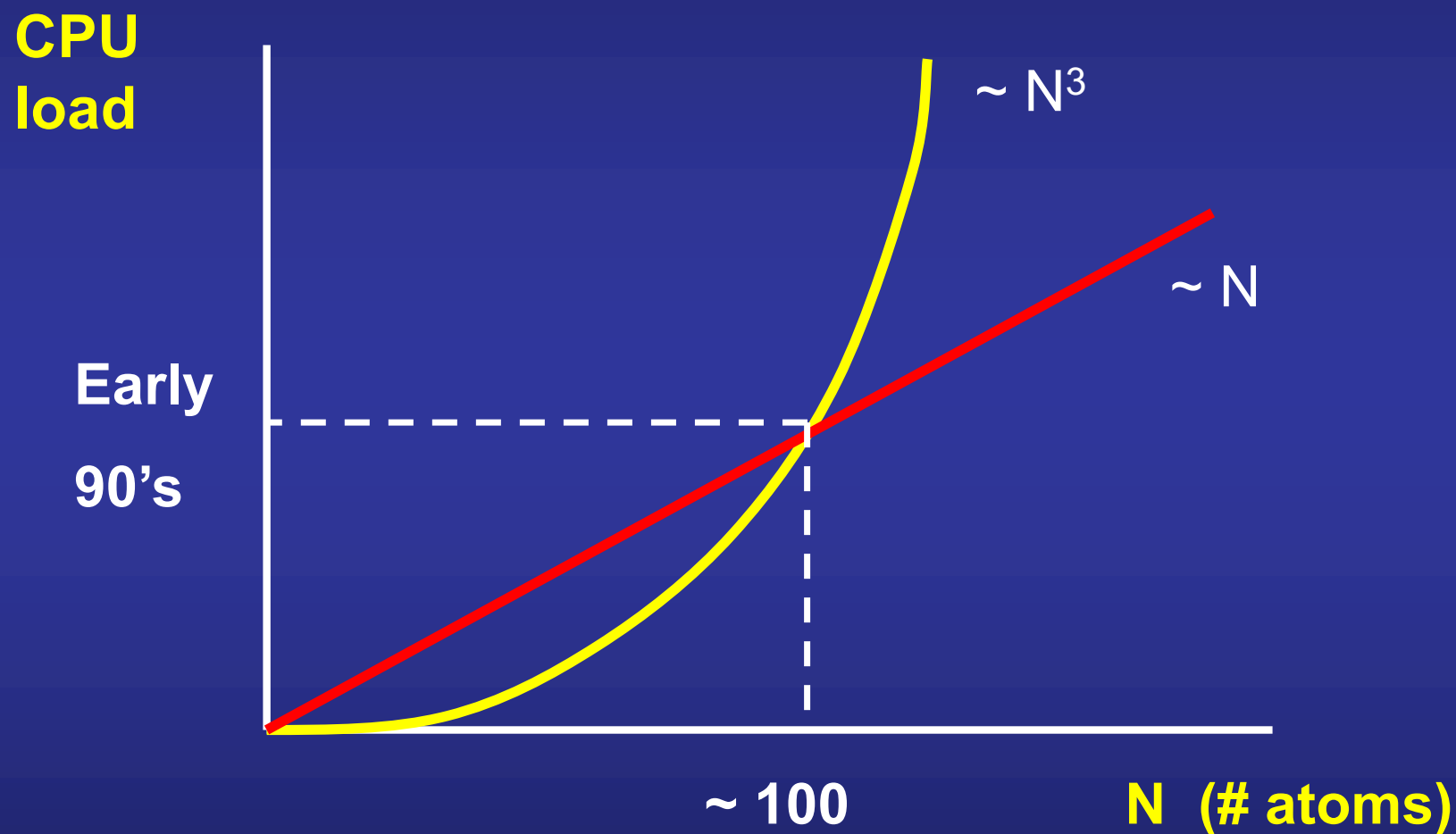
(And many more, apologize if some are missing here...)

Aim from inception: **Efficiency**

To do larger simulation boxes in modest computational platforms

Pioneer fully self-consistent **LINEAR-SCALING DFT code (or Order-N)**

Order-N methods: The computational load scales linearly with the system size



G. Galli and M. Parrinello, Phys. Rev Lett. 69, 3547 (1992)

Based on atomic-like orbitals as basis sets (LCAO: Linear Combination of Atomic Orbitals)

$$\psi_i(\vec{r}) = \sum_{\mu} \phi_{\mu}(\vec{r}) c_{\mu i} \quad \mu \equiv \{I l m n\}$$

$$\phi_{I l m n}(\vec{r}) = R_{I l n}(|\vec{r}_I|) Y_{l m}(\hat{r}_I)$$

ADVANTAGES

- **Very efficient**

(number of basis functions needed is usually very small).

Rule of thumb: 3-5 functions per electron vs ~100 PW per electron

- Large reduction of CPU time and memory
- Straightforward physical interpretation (population analysis, projected density of states,...)

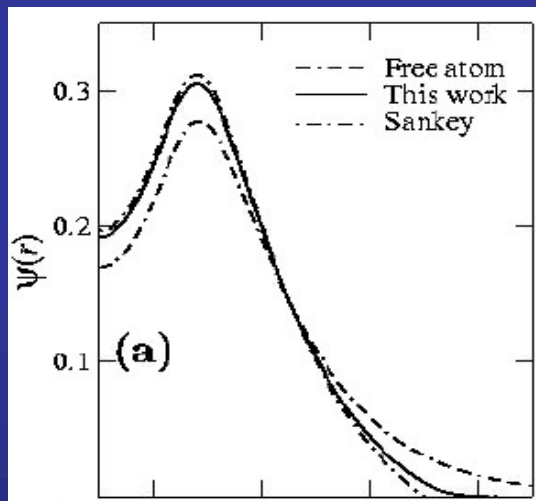
DISADVANTAGES

- ...Lack of systematic for convergence (not unique way of enlarge the basis set)
- Human and computational effort searching for a good basis set before facing a realistic project
- Responsibility on the user

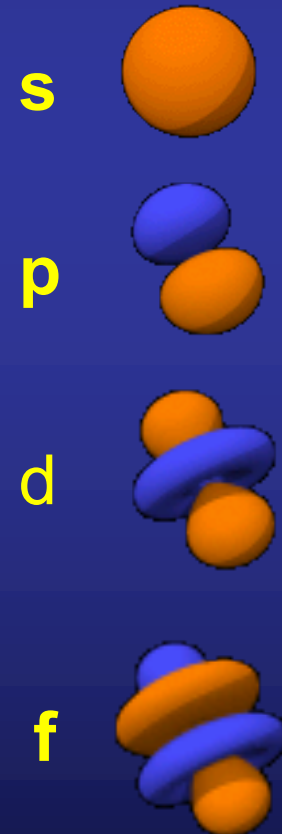
Finite support basis functions: strictly localized numerical atomic orbitals

$$\phi_{Ilmn}(\vec{r}) = R_{Ilmn}(|\vec{r}_I|) Y_{lm}(\hat{r}_I)$$

Radial part:
degree of freedom to play with



Spherical harmonics:
well defined (fixed) objects



Following Sankley and Niklewsky
Phys. Rev. B 40, 3979 (1989)

Converging the basis size: from quick and dirty to highly converged calculations

Single- ζ (minimal or SZ)

One single radial function per angular
momentum shell occupied in the free-atom

Improving the quality

```
graph TD; A[Single-ζ (minimal or SZ)] --> B[Radial flexibilization: Multiple-ζ]; A --> C[Angular flexibilization: Polarization];
```

Radial flexibilization:

Add more than one radial
function within the same angular
momentum than SZ

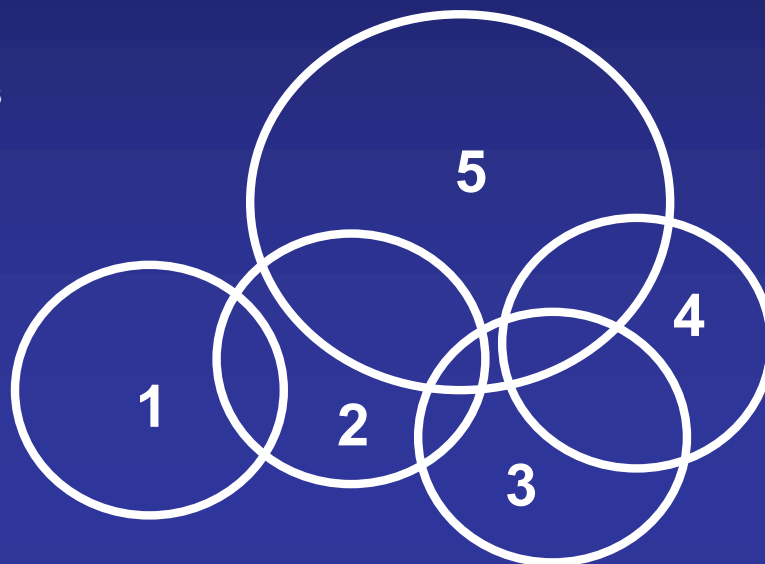
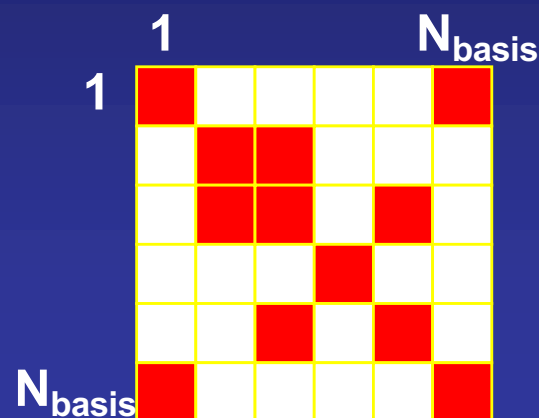
Multiple- ζ

Angular flexibilization:

Add shells of different atomic
symmetry (different l)

Polarization

Order-N methods rely heavily on the sparsity of the Hamiltonian and overlap matrices



1 with 1 and 2

2 with 1,2,3, and 5

3 with 2,3,4, and 5

4 with 3,4 and 5

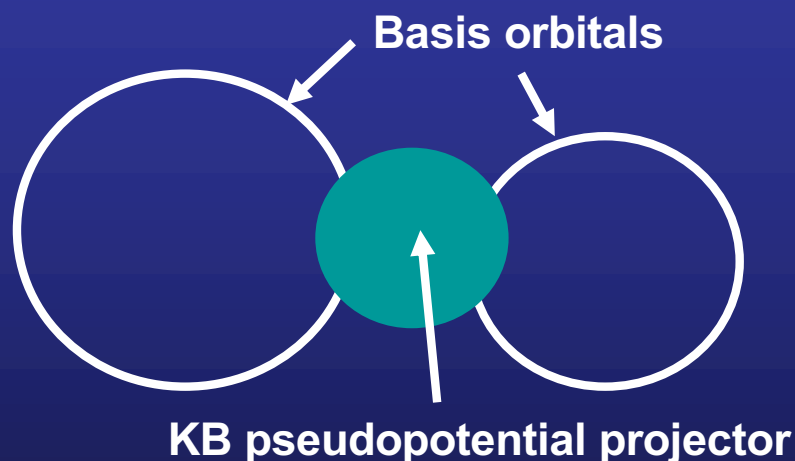
5 with 2,3,4, and 5

Sparse \equiv many entrances of the matrix are zero

$S_{\mu\nu}$ and $H_{\mu\nu}$ are sparse

$\rho_{\mu\nu}$ is not strictly sparse
but only a sparse subset
is needed

Non-overlap interactions



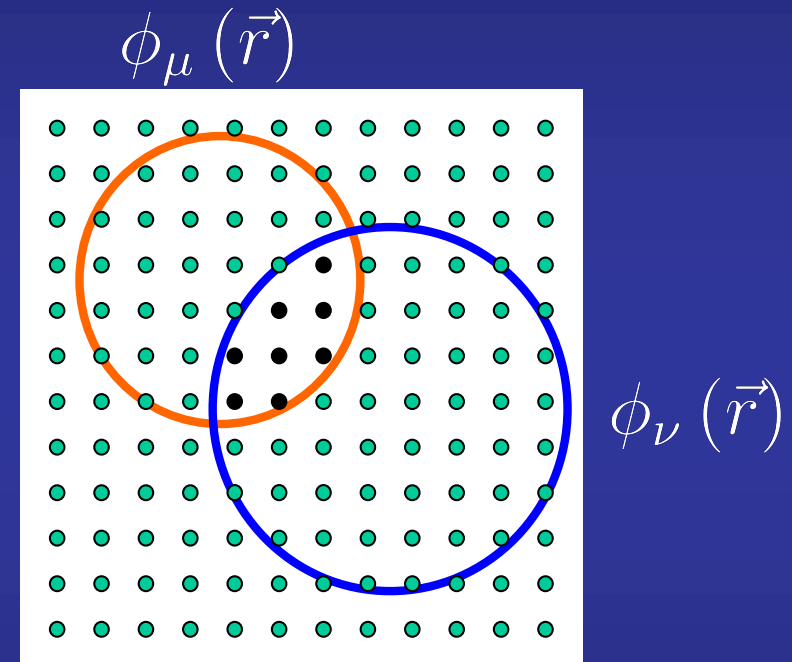
Computation of the density in real space, Hamiltonian and Overlap matrix elements: always $O(N)$

Three dimensional discrete grid to compute Hartree, exchange correlation and neutral atom potentials (related with pseudopotentials)

$$\rho(\vec{r}) = \sum_{\mu\nu} \rho_{\mu\nu} \phi_{\nu}^*(\vec{r}) \phi_{\mu}(\vec{r})$$

$$\rho_{\mu\nu} = \sum_i c_{\mu i} n_i c_{i\nu}$$

Density matrix



Find all the atomic orbitals that do not vanish at a given grid point
(in practice, interpolate the radial part from numerical tables)

Once the density is known, we compute the potentials

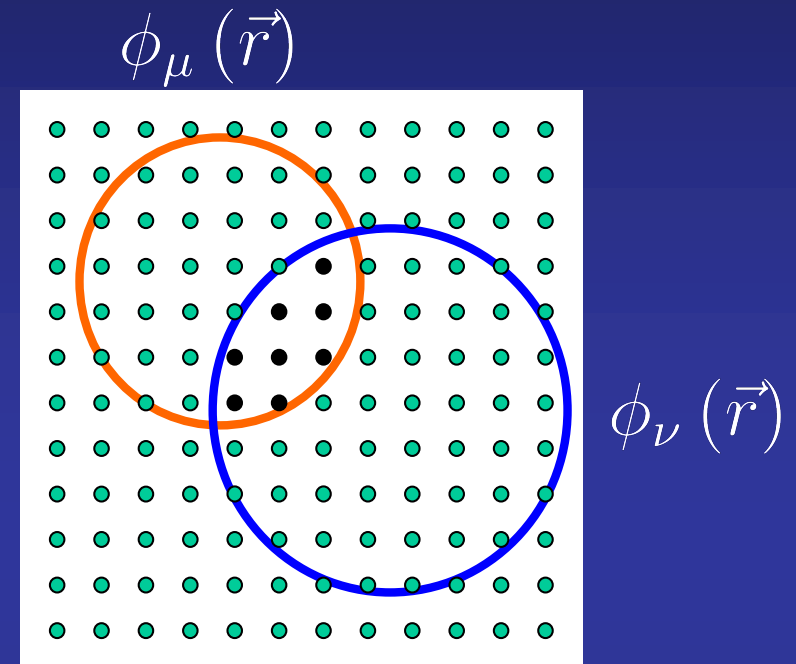
EVERYTHING $O(N)$

$$\rho(\vec{r}) \rightarrow V^{xc}(\vec{r})$$

$$\delta\rho(\vec{r}) \xrightarrow{FFT} \delta V^H(\vec{r})$$

Computation of the density in real space, Hamiltonian and Overlap matrix elements: always $O(N)$

$$\rho(\vec{r}) = \sum_{\mu\nu} \rho_{\mu\nu} \phi_{\nu}^*(\vec{r}) \phi_{\mu}(\vec{r})$$



For the computation of the Hamiltonian matrix elements,

we add together all the grid contributions and perform the integral

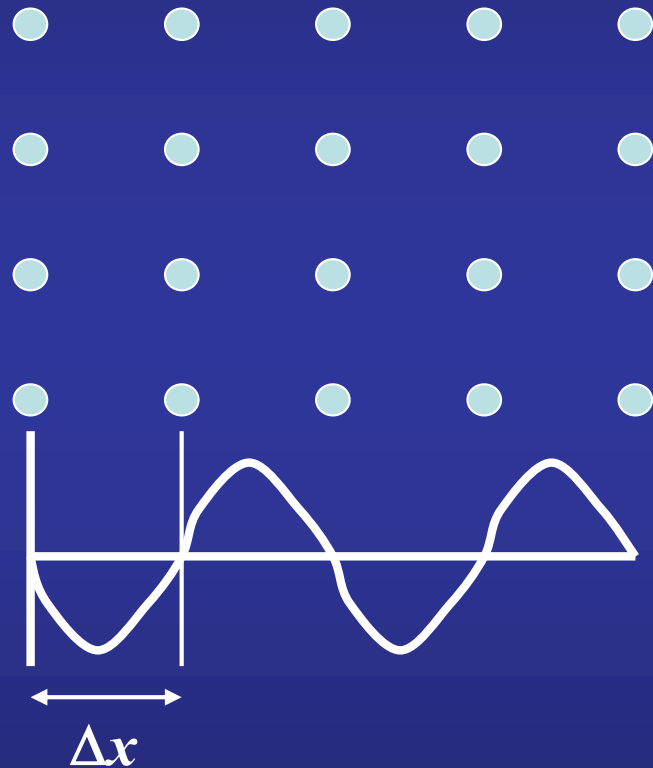
$$V(\vec{r}) = V^{NA}(\vec{r}) + \delta V^H(\vec{r}) + V^{xc}(\vec{r})$$

$$\int d\vec{r} \phi_{\nu}^*(\vec{r}) V(\vec{r}) \phi_{\nu}(\vec{r}) \approx \sum_i \phi_{\nu}^*(\vec{r}) V(\vec{r}) \phi_{\nu}(\vec{r}) \Delta\vec{r}$$

↑
Volume per grid point

Fineness of the grid controlled by a single parameter, the “MeshCutoff”

E_{cut} : maximum kinetic energy of the plane waves that can be represented in the grid without aliasing



$$\Delta x \implies k_c = \frac{\pi}{\Delta x} \implies E_c = \frac{\hbar^2 k_c^2}{2m_e}$$

In the **grid**, we represent the **density** \Rightarrow grid cutoff **not directly comparable**

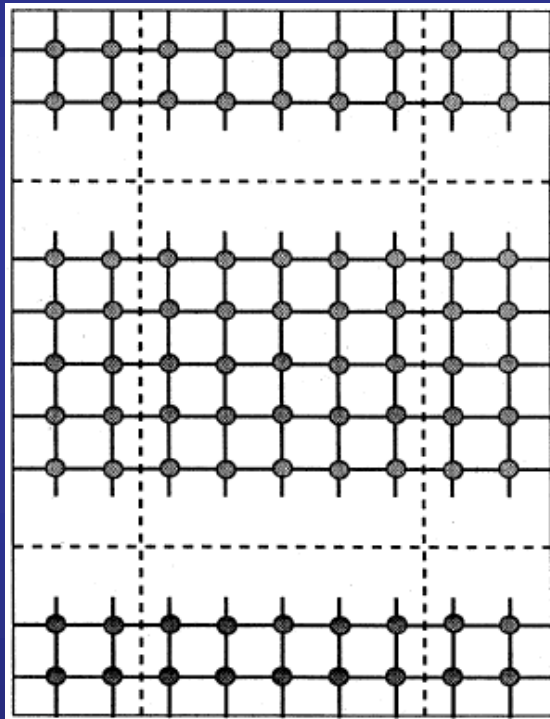
with the **plane wave cutoff** to represent wave functions

(Strictly speaking, the density requires a value four times larger)

Periodic boundary conditions. For simulations of aperiodic systems: supercell approach

Example:

The supercell approach for surfaces: the slab geometry



The semi-infinite bulk is represented by **a slab with two surfaces**

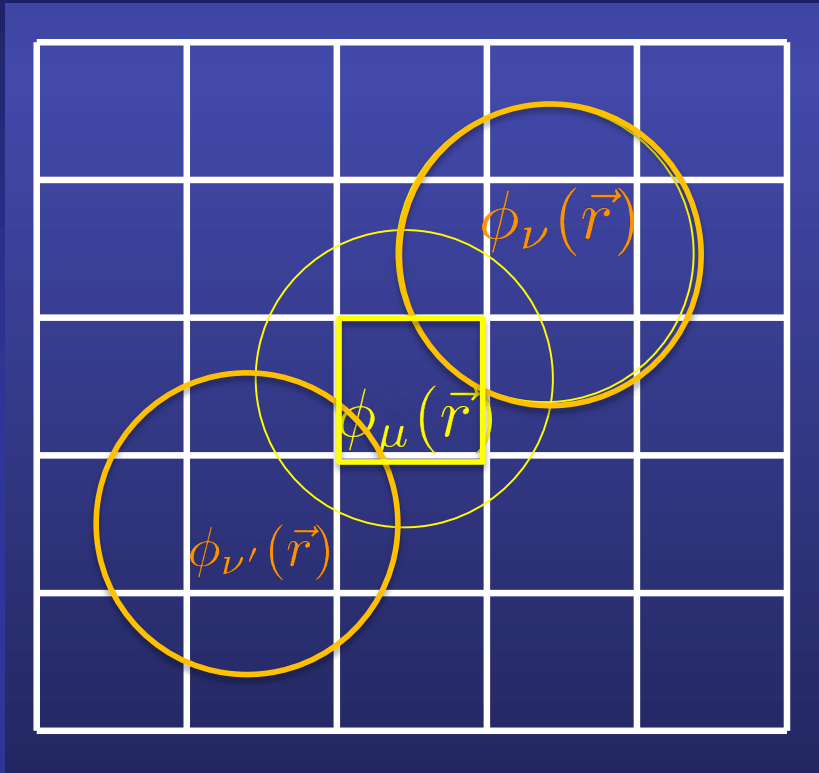
The slab has to be large enough that the two surfaces do not interact with each other

The vacuum between periodic replicas has also to be large enough, specially in charged or polarized slabs

M. C. Payne *et al.*, Rev. Mod. Phys. 64, 1045 (1992)

Usually, semiconductor and insulators require larger supercells than metals

Brillouin zone sampling



$\phi_\mu(\vec{r})$ **Orbital in the unit cell**

$\phi_\nu(\vec{r})$ and $\phi_{\nu'}(\vec{r})$
**are equivalent orbitals
related by a lattice vector**

$H_{\mu\nu'}$: **All non-zero matrix elements in real space between a
orbital in the unit cell and the periodic replicas of orbital ν**

$$H_{\mu\nu}(\vec{k}) = \sum_{\nu' \equiv \nu} H_{\mu\nu'} e^{i\vec{k} \cdot (\vec{R}_{\nu'} - \vec{R}_\mu)}$$

Once the hamiltonian and the overlap matrices are build: solve a generalized eigenvalue problem

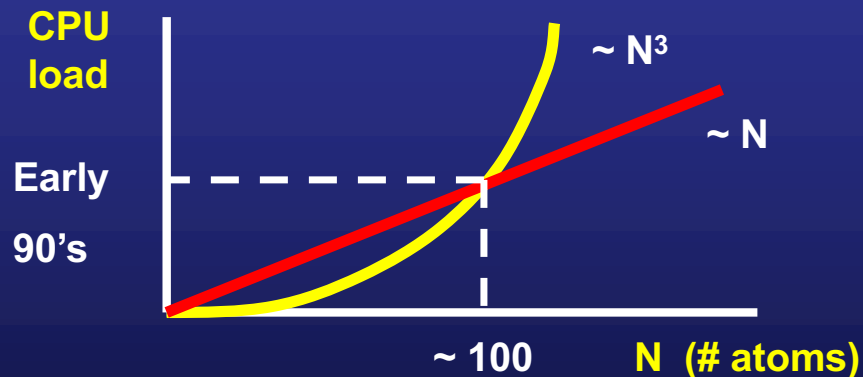
$$\begin{pmatrix} H \end{pmatrix} \begin{pmatrix} C \end{pmatrix} = E_{n\vec{k}} \begin{pmatrix} S \end{pmatrix} \begin{pmatrix} C \end{pmatrix}$$

The solver step takes most of the CPU time

Originally: linear scaling solvers

Minimization of an energy functional based on the localization of solutions

Not valid for metals or “dirty” gap systems



Now: Various solver options with various scalings

Standard diagonalization techniques:

- use pre-packaged libraries (scalapack)
- $O(N^3)$ in time, $O(N^2)$ in memory
- Both eigenvectors and eigenvalues

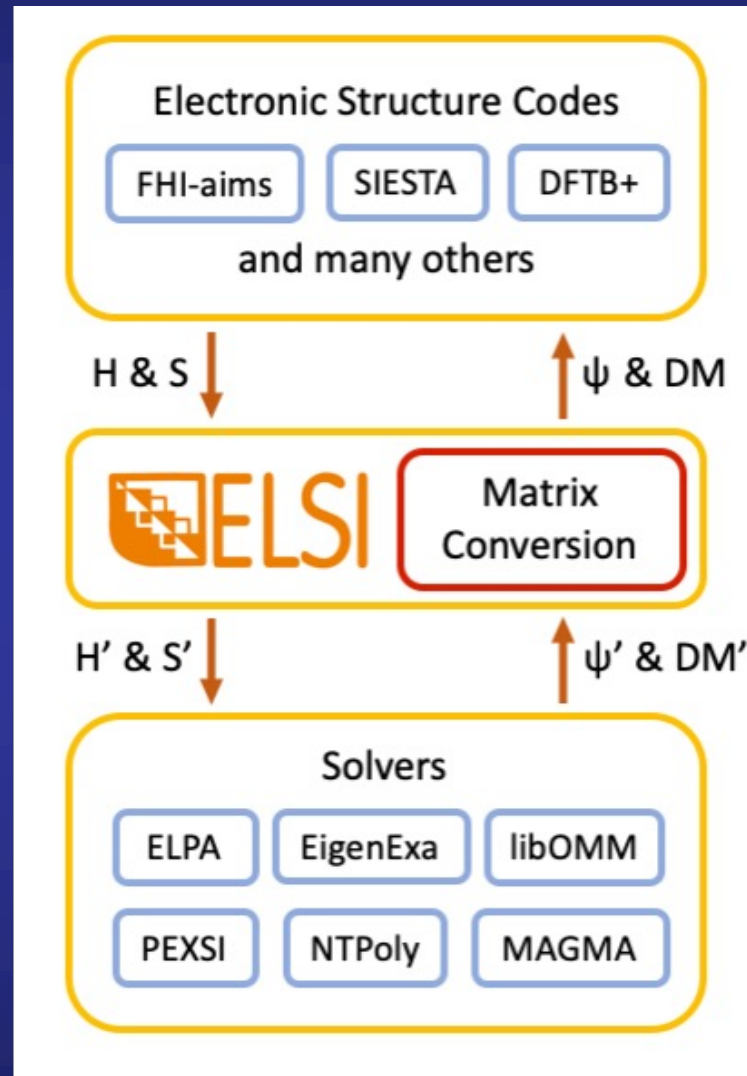
ELPA

CHESS

PEXSI

Many others

Solver structure for performance and features: Use external libraries

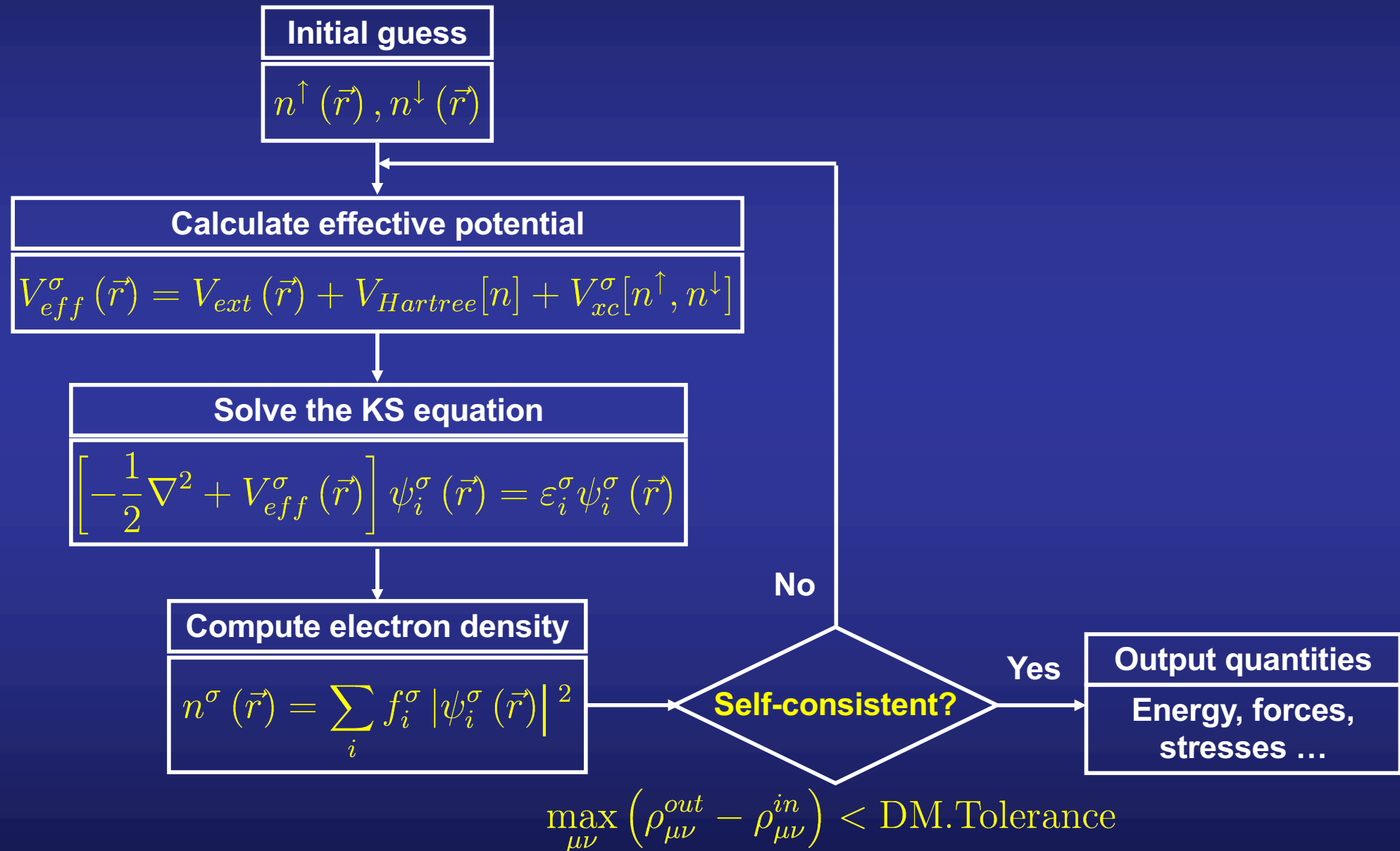


<https://elsi-interchange.org>

Interface with SIESTA: collaboration with Victor Yu (Duke University)

The Kohn-Sham equations must be solved self-consistently

The potential (input) depends on the density (output)



Atomic forces and stresses obtained by direct differentiation of the energy expression

$$\vec{F}_I = - \frac{\partial E^{KS}}{\partial \vec{R}_I}$$

$$\sigma_{\alpha\beta} = \frac{\partial E^{KS}}{\partial \epsilon_{\alpha\beta}} \quad \epsilon_{\alpha\beta} \equiv \text{strain tensor}$$

“One piece of energy \Rightarrow one piece of force and stress”

Calculated as the **analytical derivatives** of the energy

Pulay corrections, related with the dependency of the basis set on atomic positions, **automatically included**

Calculated **only** in the **last self-consistent step**

Different ensembles, different Lagrangians, different Conserved magnitudes.

- *NVE (Verlet):
Microcanonical.*
- *Integrates Newtons equations of motion, for N particles, in a fixed volume V.*
- *Natural time evolution of the system:
E is a constant of motion*

- *NVT (Nose): Canonical*
- *System in thermal contact with a heat bath.*
- *Extended Lagrangian:*
- *N particles + Thermostat, mass Q.*

- *NPE (Parrinello-Rahman)
(isobarical)*
- *Extended Lagrangian*
- *Cell vectors are dynamical variables with an associated mass.*

- *NPT (Nose-Parrinello-Rahman)*
- *2 Extended Lagrangians*
- *NVT+NPE.*

SIESTA capabilities

SIESTA: Recent developments and applications

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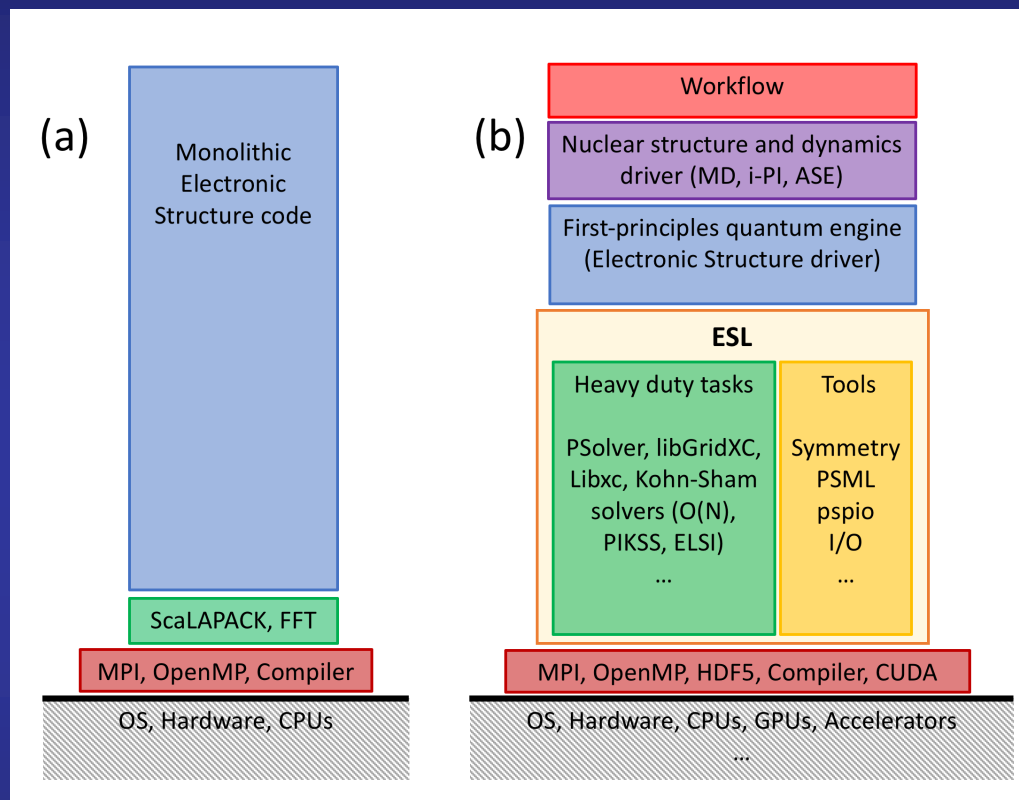


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and Javier Junquera^{15,aj)}

- PSML pseudopotentials
- LDA+U
- TRANSIESTA (ballistic charge transport at the nanoscale)
- TDDFT in real time
- Full Spin-Orbit coupling, non-collinear magnetism
- Various eigensolvers with different scalings
- Density functional perturbation theory
- TDDFT in frequency space and GW post-processing
- Multiscale (second-principles) and QM/MM
- Several analysis and post-processing tools
- Wannierization
- Hybrid functionals
- Dynamical Mean Field Theory (coming soon)
- Superconductivity and electron phonon coupling

SIESTA modularity: A change in the paradigm

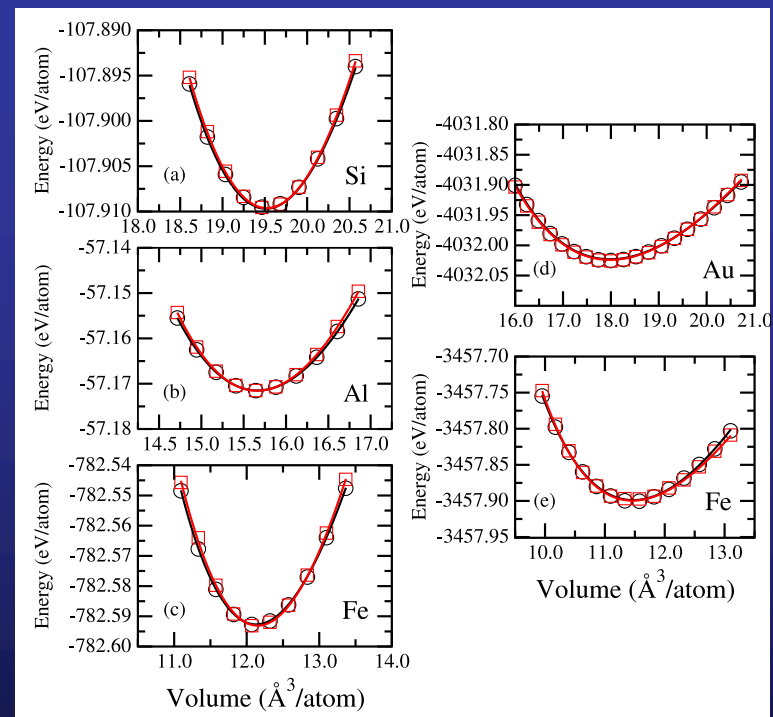
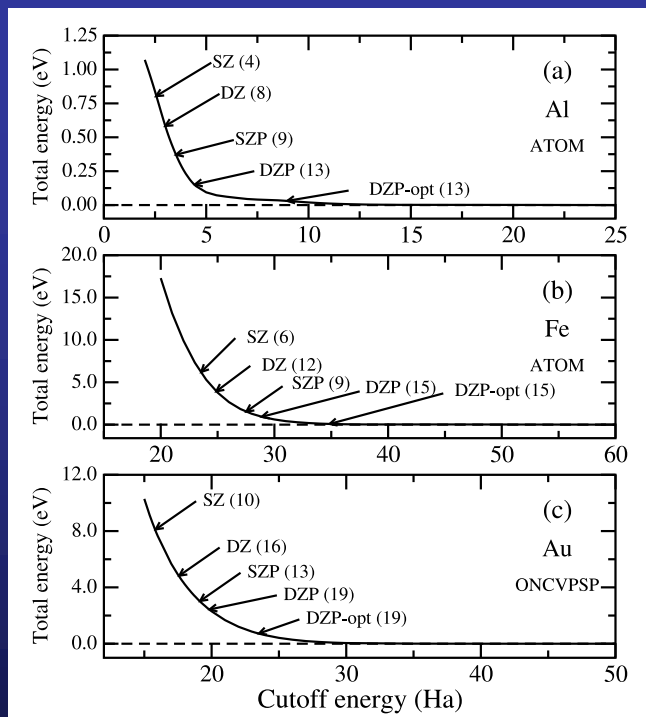


The CECAM electronic structure library

M. J. T. Oliveira *et al.*
J. Chem. Phys. 153, 024117 (2020)

Norm conserving pseudopotential library in Pseudopotential Markup Language (PSML) format

Remove interoperability problems
(the same pseudopotential operator can be used by different codes)



Norm conserving pseudopotential library in Pseudopotential Markup Language (PSML) format

<http://www.pseudo-dojo.org>

The screenshot displays the Pseudo-Dojo website interface. At the top, there's a logo and the text "PSEUDO DOJO". Below this, a "Download" button is visible. A sidebar on the left contains a "Help me" button and a small periodic table. The main area features a large periodic table where each element's box contains its symbol, atomic number, and a 3x3 matrix of pseudopotential values. Above the table, there are tabs for "Type", "XC", "Accuracy", and "Format". The "Format" tab is currently selected, showing "psml". To the right of the table, there's a "F.A.Q. Contribute Papers About" section and a "Select the flavor and format, then click 'Download' to get the complete table of pseudos or choose a specific element. 'HTML' gives full test results." section. Below this, there's a small table of element symbols and their corresponding pseudopotential values.

Help me

PSEUDO DOJO

Download

3.13 Mean

hints tests

32.74 0.95

37.25 2.20

43.36 -0.09

F.A.Q. Contribute Papers About

Select the flavor and format, then click "Download" to get the complete table of pseudos or choose a specific element. "HTML" gives full test results.

2 He 1

39 45 49 na

4.2 4.2 na

Helium

5 B 2

34 38 44 0.3 0.8 0.1

0.1 0.1 0.1

0.1 0.1 0.1

Boron

6 C 2

37 41 45 0.1 0.1 0.1

0.1 0.1 0.1

0.1 0.1 0.1

Carbon

7 N 2

36 42 48 0.2 0.4 0.4

0.4 0.4 0.4

0.4 0.4 0.4

Nitrogen

8 O 2

36 42 48 2.0 6.5 6.5

6.5 6.5 6.5

6.5 6.5 6.5

Oxygen

9 F 2

36 42 48 0.1 0.6 0.6

0.6 0.6 0.6

0.6 0.6 0.6

Fluorine

10 Ne 2

30 34 40 na

1.7 1.7 na

1.7 1.7 na

Neon

11 Na 3

38 44 48 0.4 1.6 1.6

1.6 1.6 1.6

1.6 1.6 1.6

Sodium

12 Mg 3

38 44 48 0.4 1.5 1.5

1.5 1.5 1.5

1.5 1.5 1.5

Magnesium

Type

NC SR (ONCVSP v0.4.1)

XC

PBE

Accuracy

standard

Format

psml

13 Al 2

16 20 26 0.5 1.3 1.3

1.3 1.3 1.3

1.3 1.3 1.3

Aluminum

14 Si 2

14 18 24 0.1 0.2 0.2

0.2 0.2 0.2

0.2 0.2 0.2

Silicon

15 P 2

18 22 28 0.1 0.3 0.3

0.3 0.3 0.3

0.3 0.3 0.3

Phosphorus

16 S 2

20 24 32 0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

Sulphur

17 Cl 2

25 33 37 0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

Chlorine

18 Ar 2

29 33 37 na

0.0 0.0 na

0.0 0.0 na

Argon

19 K 3

33 37 43 0.2 2.0 2.0

2.0 2.0 2.0

2.0 2.0 2.0

Potassium

20 Ca 3

28 34 40 0.1 0.3 0.3

0.3 0.3 0.3

0.3 0.3 0.3

Calcium

21 Sc 4

35 41 47 1.3 1.3 1.3

1.3 1.3 1.3

1.3 1.3 1.3

Scandium

22 Ti 4

38 42 48 1.3 1.3 1.3

1.3 1.3 1.3

1.3 1.3 1.3

Titanium

23 V 4

42 46 52 1.3 1.3 1.3

1.3 1.3 1.3

1.3 1.3 1.3

Vanadium

24 Cr 4

42 46 52 1.3 1.3 1.3

1.3 1.3 1.3

1.3 1.3 1.3

Chromium

25 Mn 4

42 46 52 1.3 1.3 1.3

1.3 1.3 1.3

1.3 1.3 1.3

Manganese

26 Fe 4

42 46 52 5.6 5.6 5.6

5.6 5.6 5.6

5.6 5.6 5.6

Iron

27 Co 4

42 46 52 1.0 1.0 1.0

1.0 1.0 1.0

1.0 1.0 1.0

Cobalt

28 Ni 4

45 49 55 1.1 1.1 1.1

1.1 1.1 1.1

1.1 1.1 1.1

Nickel

29 Cu 4

42 46 52 0.5 0.5 0.5

0.5 0.5 0.5

0.5 0.5 0.5

Copper

30 Zn 4

38 42 48 0.8 0.8 0.8

0.8 0.8 0.8

0.8 0.8 0.8

Zinc

31 Ga 3

36 40 44 0.5 1.5 1.5

1.5 1.5 1.5

1.5 1.5 1.5

Gallium

32 Ge 3

36 40 44 0.5 1.0 1.0

1.0 1.0 1.0

1.0 1.0 1.0

Germanium

33 As 3

36 40 44 0.4 0.7 0.7

0.7 0.7 0.7

0.7 0.7 0.7

Arsenic

34 Se 3

36 40 44 0.2 0.5 0.5

0.5 0.5 0.5

0.5 0.5 0.5

Selenium

35 Br 2

36 40 44 0.2 0.5 0.5

0.5 0.5 0.5

0.5 0.5 0.5

Bromine

36 Kr 2

22 26 34 na

0.0 0.0 na

0.0 0.0 na

Krypton

37 Rb 3

23 27 33 0.2 2.9 2.9

2.9 2.9 2.9

2.9 2.9 2.9

Rubidium

38 Sr 3

28 34 40 0.1 0.3 0.3

0.3 0.3 0.3

0.3 0.3 0.3

Strontium

39 Y 3

36 42 48 1.0 1.0 1.0

1.0 1.0 1.0

1.0 1.0 1.0

Yttrium

40 Zr 4

33 37 43 1.1 1.1 1.1

1.1 1.1 1.1

1.1 1.1 1.1

Zirconium

41 Nb 4

37 41 47 1.3 1.3 1.3

1.3 1.3 1.3

1.3 1.3 1.3

Niobium

42 Mo 4

36 40 44 1.4 1.4 1.4

1.4 1.4 1.4

1.4 1.4 1.4

Molybdenum

43 Tc 4

38 42 48 1.6 1.6 1.6

1.6 1.6 1.6

1.6 1.6 1.6

Technetium

44 Ru 4

38 42 48 2.1 2.1 2.1

2.1 2.1 2.1

2.1 2.1 2.1

Ruthenium

45 Rh 4

40 44 50 2.6 2.6 2.6

2.6 2.6 2.6

2.6 2.6 2.6

Rhodium

46 Pd 3

37 41 47 1.1 1.1 1.1

1.1 1.1 1.1

1.1 1.1 1.1

Palladium

47 Ag 4

37 41 47 0.3 0.3 0.3

0.3 0.3 0.3

0.3 0.3 0.3

Silver

48 Cd 4

37 41 47 1.1 1.1 1.1

1.1 1.1 1.1

1.1 1.1 1.1

Cadmium

49 In 3

31 35 41 0.1 0.2 0.2

0.2 0.2 0.2

0.2 0.2 0.2

Indium

50 Sn 3

32 36 42 0.8 0.8 0.8

0.8 0.8 0.8

0.8 0.8 0.8

Tin

51 Sb 3

36 40 44 0.5 1.0 1.0

1.0 1.0 1.0

1.0 1.0 1.0

Antimony

52 Te 3

34 38 44 0.8 0.8 0.8

0.8 0.8 0.8

0.8 0.8 0.8

Tellurium

53 I 2

34 38 44 1.1 1.1 1.1

1.1 1.1 1.1

1.1 1.1 1.1

Iodine

54 Xe 2

28 32 36 0.0 0.0 0.0

0.0 0.0 0.0

0.0 0.0 0.0

Xenon

55 Cs 3

19 23 29 0.1 1.5 1.5

1.5 1.5 1.5

1.5 1.5 1.5

Caesium

56 Ba 3

18 22 28 0.9 4.9 4.9

4.9 4.9 4.9

4.9 4.9 4.9

Barium

57 La 4

50 54 58 na

na na na

na na na

Lanthanum

58 Ce na

na na na

na na na

na na na

Cerium

59 Pr na

na na na

na na na

na na na

Praseodymium

60 Nd na

na na na

na na na

na na na

Neodymium

61 Pm na

na na na

na na na

na na na

Promethium

62 Sm na

na na na

na na na

na na na

Samarium

63 Eu na

na na na

na na na

na na na

Europium

64 Gd na

na na na

na na na

na na na

Gadolinium

65 Tb na

na na na

na na na

na na na

Terbium

66 Dy na

na na na

na na na

na na na

Dysprosium

67 Ho na

na na na

na na na

na na na

Holmium

68 Er na

na na na

na na na

na na na

Erbium

69 Tm na

na na na

na na na

na na na

Thulium

70 Yb na

na na na

na na na

na na na

Ytterbium

71 Lu 5

46 50 54 1.0 2.2 2.2

2.2 2.2 2.2

2.2 2.2 2.2

Lutetium

89 Ac

90 Th

91 Pa

92 U

93 Np

94 Pu

95 Am

96 Cm

97 Bk

98 Cf

99 Es

100 Fm

101 Md

102 No

103 Lr

Actinium

Thorium

Protactinium

Uranium

Neptunium

Plutonium

Americium

Curium

Berkelium

Californium

Einsteinium

Fermium

Mendelevium

Nobelium

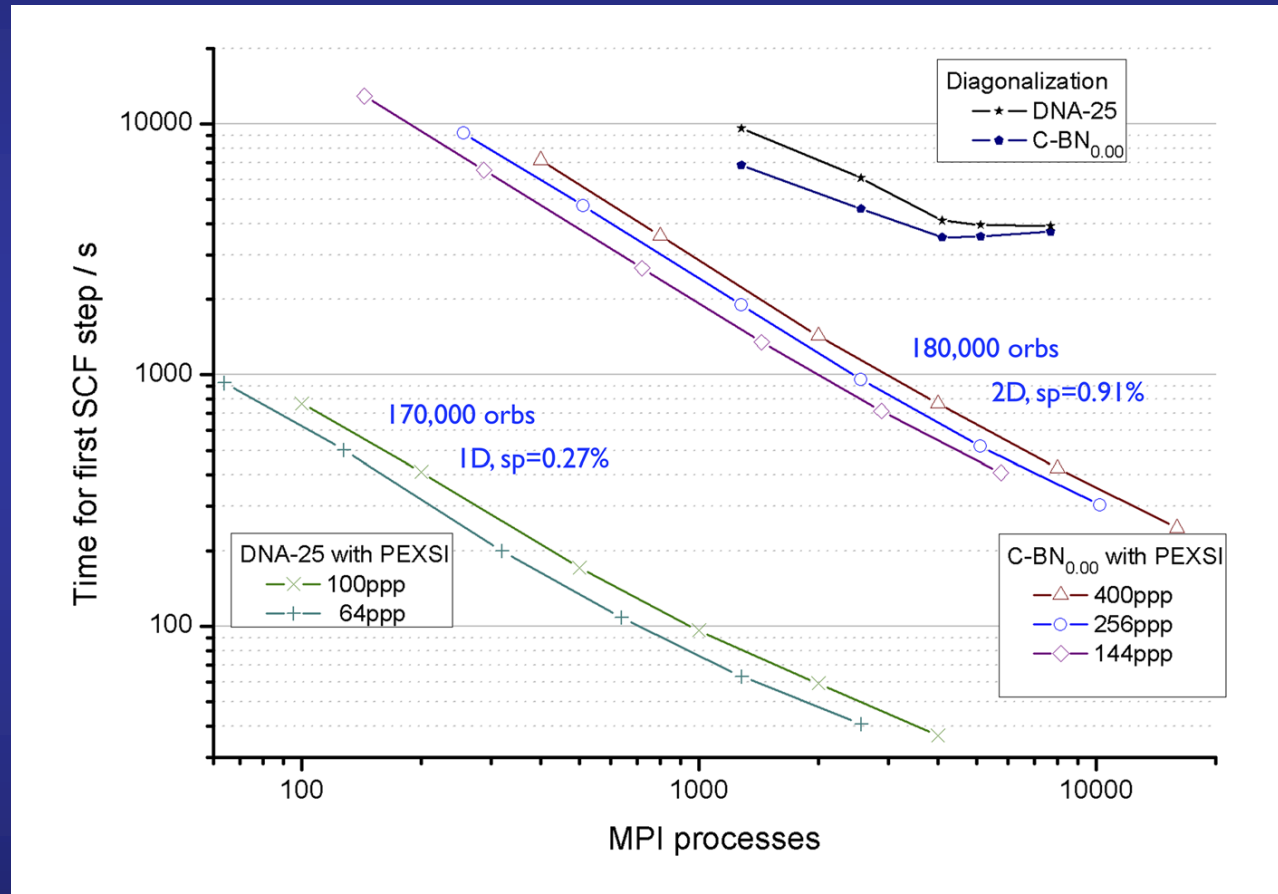
Lawrencium

Periodic table of curated pseudopotentials

The **testing** of the pseudopotential is a **responsability of the user**,
But the availability of reliable and accurate norm-conserving
pseudopotential lowers the barrier

SIESTA parallelization

Both distributed [message-passing (MPI)] and shared-memory (OpenMP) parallelization options implemented



SIESTA base line efficiency can be scaled up to every larger systems

SIESTA is a very user friendly code

```
SystemName          Water molecule
SystemLabel         h2o
NumberOfAtoms       3
NumberOfSpecies     2

%block ChemicalSpeciesLabel
  1  8  0      # Species index, atomic number, species label
  2  1  H
%endblock ChemicalSpeciesLabel

AtomicCoordinatesFormat Ang
%block AtomicCoordinatesAndAtomicSpecies
  0.000  0.000  0.000  1
  0.757  0.586  0.000  2
 -0.757  0.586  0.000  2
%endblock AtomicCoordinatesAndAtomicSpecies
```

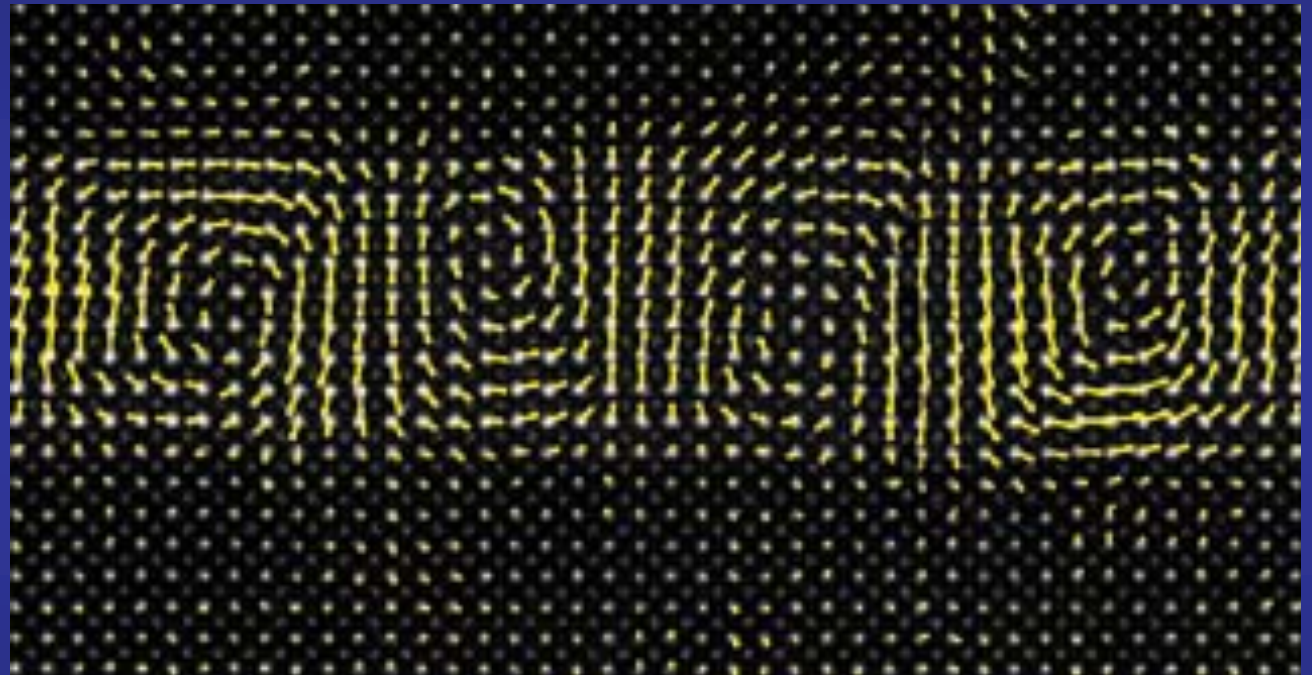
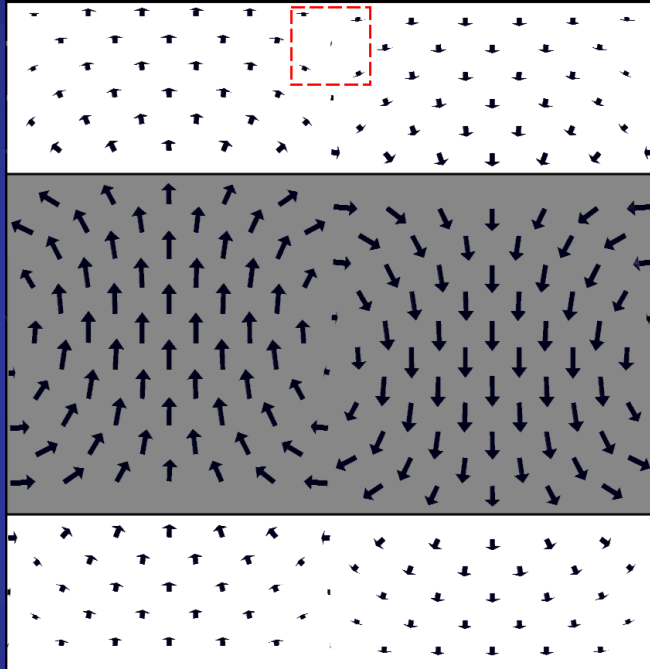
SIESTA applications in extremely varied contexts

- Physics
- Chemistry
- Material Science
- Biology
- Geology
- Nanoscience
- Engineering
- Pharmacy

Difficult to follow (over 2000 citations per year)

<input type="checkbox"/>	The SIESTA method for ab initio order-N materials simulation JM Soler, E Artacho, JD Gale, A García, J Junquera, P Ordejón, ... Journal of Physics: Condensed Matter 14 (11), 2745	11746	2002
	Density-functional method for nonequilibrium electron transport M Brandbyge, JL Mozos, P Ordejón, J Taylor, K Stokbro Physical Review B 65 (16), 165401	4806	2002
	Self-consistent order-N density-functional calculations for very large systems P Ordejón, E Artacho, JM Soler Physical Review B 53 (16), R10441	2788	1996
	Density-functional method for very large systems with LCAO basis sets D Sánchez-Portal, P Ordejón, E Artacho, JM Soler International journal of quantum chemistry 65 (5), 453-461	1851	1997
	Linear-scaling ab-initio calculations for large and complex systems E Artacho, D Sánchez-Portal, P Ordejón, A Garcia, JM Soler physica status solidi (b) 215 (1), 809-817	1181	1999
<input type="checkbox"/>	Numerical atomic orbitals for linear-scaling calculations J Junquera, Ó Paz, D Sánchez-Portal, E Artacho Physical Review B 64 (23), 235111	1133	2001
<input type="checkbox"/>	The SIESTA method; developments and applicability E Artacho, E Anglada, O Diéguez, JD Gale, A García, J Junquera, ... Journal of Physics: Condensed Matter 20 (6), 064208	599	2008
<input type="checkbox"/>	Systematic generation of finite-range atomic basis sets for linear-scaling calculations E Anglada, JM Soler, J Junquera, E Artacho Physical Review B 66 (20), 205101	318	2002

Material science: topologically non-trivial phases in $\text{PbTiO}_3/\text{SrTiO}_3$ superlattices

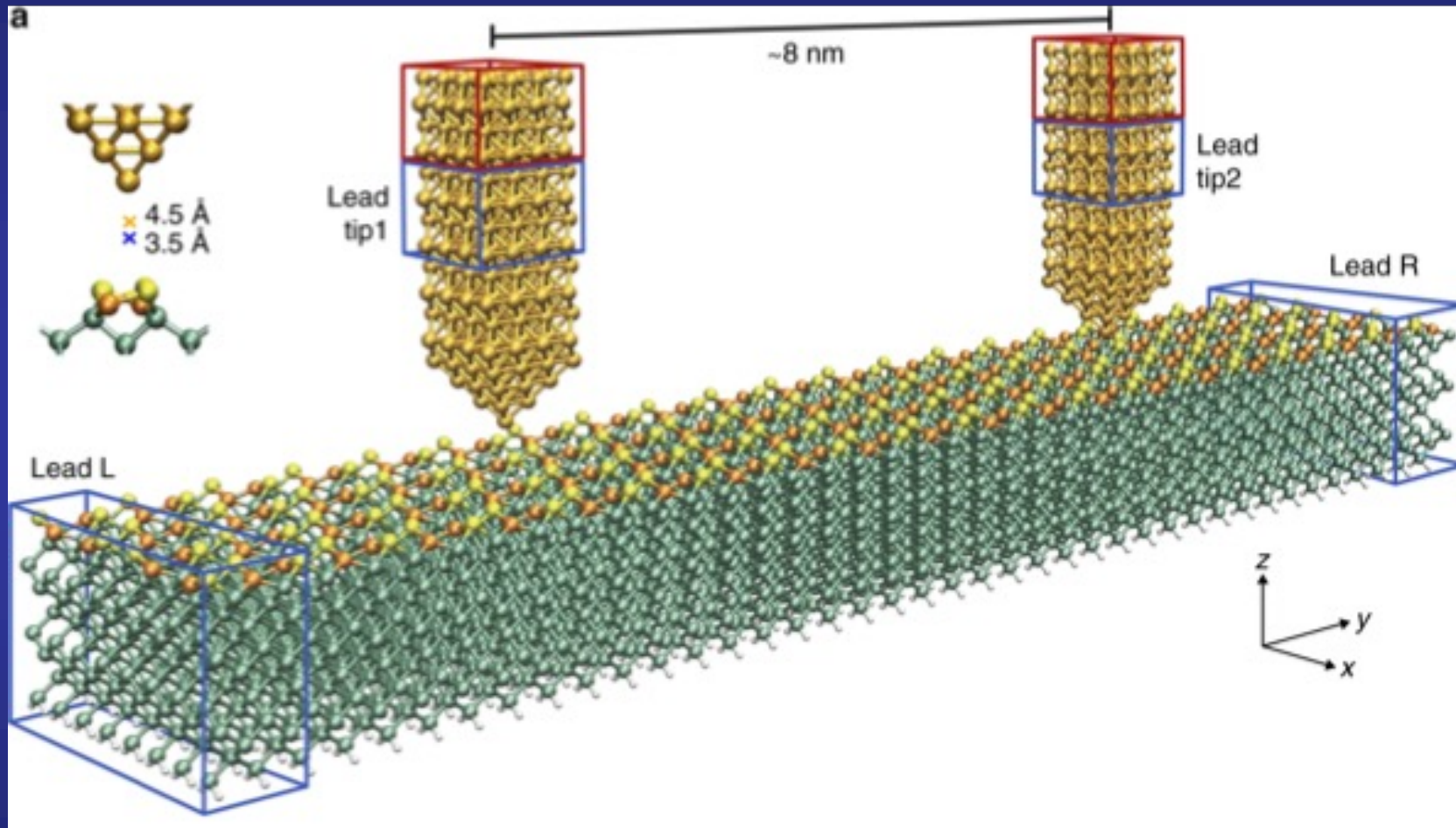


P. Aguado-Puente and J. Junquera
Phys. Rev. B 85, 184105 (2012)

A. Yadav *et al.* Nature 530, 198 (2016)

Predictive power of the simulations

Nanotechnology: quantum mechanical transport simulations

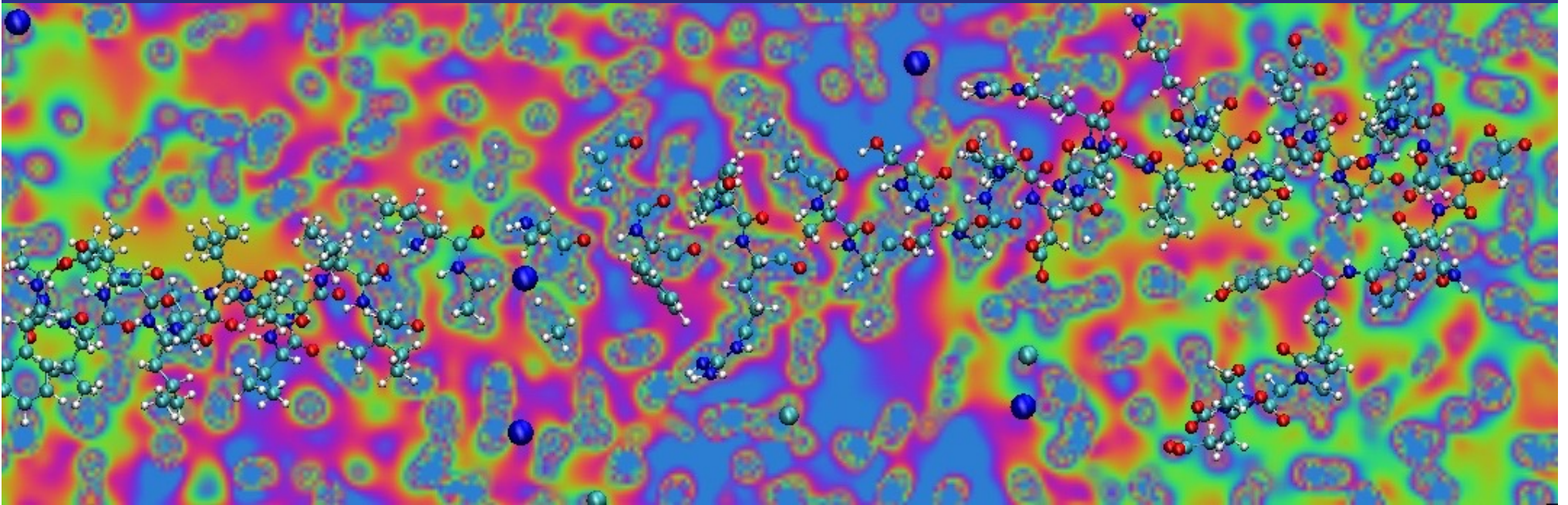


Four terminal transport on Ge Surface and gold tips
(4924 atoms)

M. Kolmer *et al.* Nat. Commun. 10, 1573 (2019)

Biology:

Electrostatics around pilin protein in wet conditions



A natural nano electric wire
(4580 atoms)

G. T. Feliciano *et al.* J. Phys. Chem. A 116, 8023 (2012)

Distribution: fully open source (GPL) since 2016

<http://gitlab.com/siesta-project>

The screenshot displays the GitLab web interface for the 'siesta-project' group. The top navigation bar includes the GitLab logo and links for Projects, Groups, Snippets, and Help. A search bar and a 'Sign in / Register' button are also present. The left sidebar shows the 'siesta-project' group overview with links to Details, Activity, Issues (69), Merge requests (26), Packages & Registries, and Members. The main content area shows the 'siesta-project' group details, including its description: 'First-principles materials simulation using Siesta and related tools'. Below this, there are tabs for 'Subgroups and projects', 'Shared projects', and 'Archived projects'. The 'Subgroups and projects' tab is active, showing a list of subgroups and projects. The subgroups listed are 'analysis-tools' (A subgroup of Siesta-Project to deal with analysis tools) and 'Libraries' (Libraries originating in the Siesta project). The 'analysis-tools' subgroup has 0 folders, 5 bookmarks, and 1 member. The 'Libraries' subgroup has 0 folders, 6 bookmarks, and 1 member. At the bottom, there is a project entry for 'siesta' (A first-principles materials simulation code using DFT. Homepage: <https://siesta-pr...>) with 31 stars and a creation date of 1 month ago.

GitLab Projects Groups Snippets Help Search or jump to... Sign in / Register

siesta-project

Group overview Details Activity

Issues 69 Merge requests 26 Packages & Registries Members

siesta-project Group ID: 4376285

First-principles materials simulation using Siesta and related tools

Subgroups and projects Shared projects Archived projects Search by name Name

> analysis-tools A subgroup of Siesta-Project to deal with analysis tools 0 5 1

> Libraries Libraries originating in the Siesta project. 0 6 1

siesta A first-principles materials simulation code using DFT. Homepage: <https://siesta-pr...> 31 1 month ago

Siesta support

<https://departments.icmab.es/leem/siesta/>



[Home](#) [About](#) [Code](#) [Documentation](#) [Pseudopotentials](#) [The Team](#) [News](#) [Support](#)

SIESTA is both a method and its computer program implementation, to perform efficient electronic structure calculations and ab initio molecular dynamics simulations of molecules and solids. SIESTA's efficiency stems from the use of a basis set of strictly-localized atomic orbitals. A very important feature of the code is that its accuracy and cost can be tuned in a wide range, from quick exploratory calculations to highly accurate simulations matching the quality of other approaches, such as plane-wave methods.

The possibility of treating large systems with some first-principles electronic-structure methods has opened up new opportunities in many disciplines. The SIESTA program is open source and has become quite popular, being increasingly used by researchers in geosciences, biology, and engineering (apart from those in its natural habitat of materials physics and chemistry). Currently there are several thousand users all over the world, and the paper describing the method ([J. Phys. Cond. Matt. 14, 2745 \(2002\)](#)) has received more than 8000 citations so far.

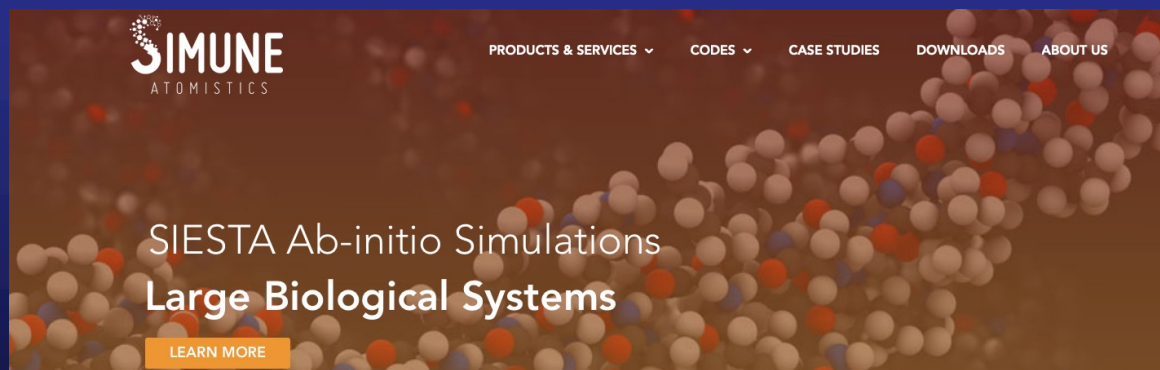
For an overview of recent developments, and sample applications of SIESTA, see [J. Chem. Phys. 152, 204108 \(2020\)](#).

SIESTA is one of the flagship codes of the [MaX Center of Excellence](#).

Devoted **Youtube channel** will be launched **next week**

SIMUNE: a Company that offers profesional support

<https://www.simuneatomistics.com>



Siesta support

<https://personales.unican.es/junqueraj/siesta-tutorial.html>

Self-explained SIESTA tutorial

Updated April 2016

Here we present a collection of theoretical lectures and self-explained SIESTA exercises compiled during the years on many schools and tutorials. I would like to acknowledge the collaboration of the SIESTA team during the preparation, testing, and cleaning of the exercises:

Emilio Artacho	CIC Nanogune	San Sebastián (Spain)
Julian Gale	Curtin University of Technology	Perth (Australia)
Alberto García	Institut de Ciència de Materials de Barcelona (ICMAB-CSIC)	Barcelona (Spain)
José Soler	Universidad Autónoma de Madrid	Madrid (Spain)
Pablo Ordejón	Institut Català de Nanociència i Nanotecnologia (ICN2)	Barcelona (Spain)
Daniel Sánchez-Portal	Unidad de Física de Materiales, Centro Mixto CSIC-UPV/EHU	San Sebastián (Spain)

The present exercises are just simple examples to show how-to run different capabilities of SIESTA. Before running a calculation for production, test the pseudopotentials, basis sets, and perform the convergence tests (mesh cutoff, k-grid sampling, etc). Some of these parameters have been chosen for you to speed up the calculations, and might not be converged.

Please, report any error or mistake that you could detect on these exercises to: [javier.junquera -- unican.es](mailto:javier.junquera@unican.es)

Openings

Some openings for PhD fellowships funded by the University of Cantabria are available. If you are a Master student who wish to work in the field, please take a look at [this call](#)

The Theory of Condensed Matter Group at the University of Cantabria is willing to support personal applications to PhD and post-doctoral fellowships offered by funding agencies from Spain and Europe (through the Marie Skłodowska-Curie actions)

[Some theoretical lectures](#)

[Set of self-explained SIESTA exercises](#)

[Back to Javier Junquera's home page](#)