Imperial College London

THE THOMAS YOUNG CENTRE TYC

Introduction to ONETEP

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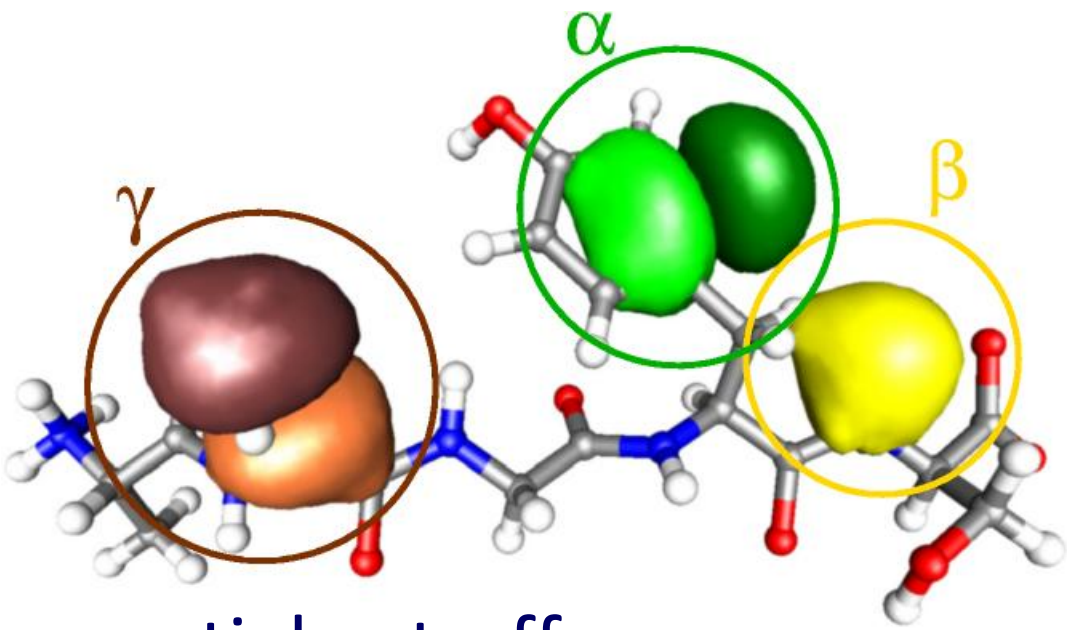
Outline

- Overview of basic concepts
- Compilation requirements
- Running a simple calculation

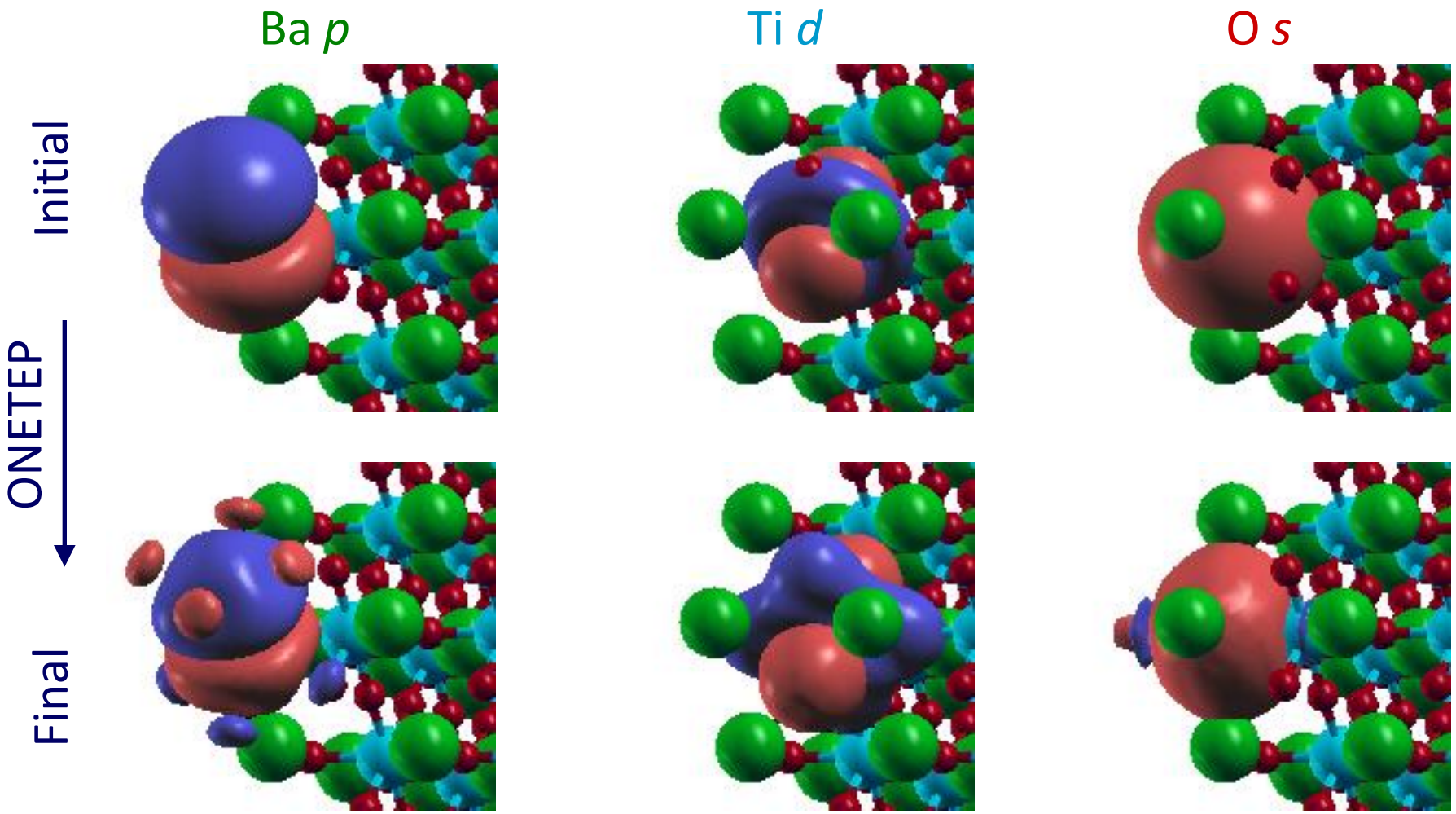
Density-matrix formulation

$$\rho(\mathbf{r},\mathbf{r}') = \sum_{\alpha\beta} \phi_\alpha(\mathbf{r}) K^{\alpha\beta} \phi_\beta(\mathbf{r}')$$



- Impose spatial cut-offs:
  - Non-orthogonal generalised Wannier functions
  - Sparse density kernel K

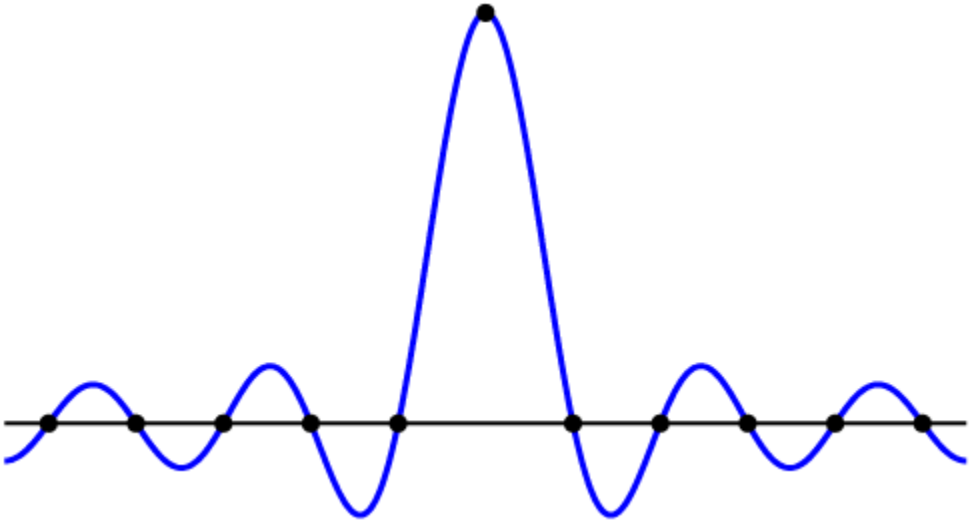
NGWF optimisation

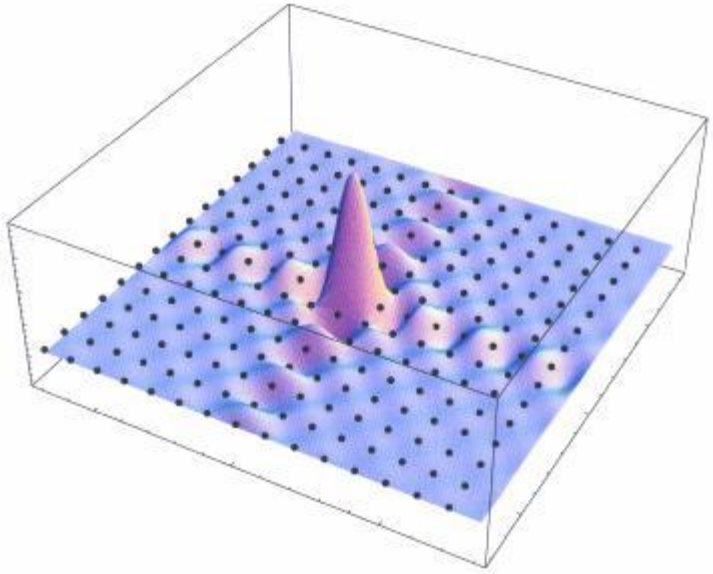


On-site rotation from Foster & Weinhold, *J. Am. Chem. Soc.* **102**, 7211 (1980)

Basis set: psincs

- "Periodic Cardinal Sine" or Dirichlet functions:

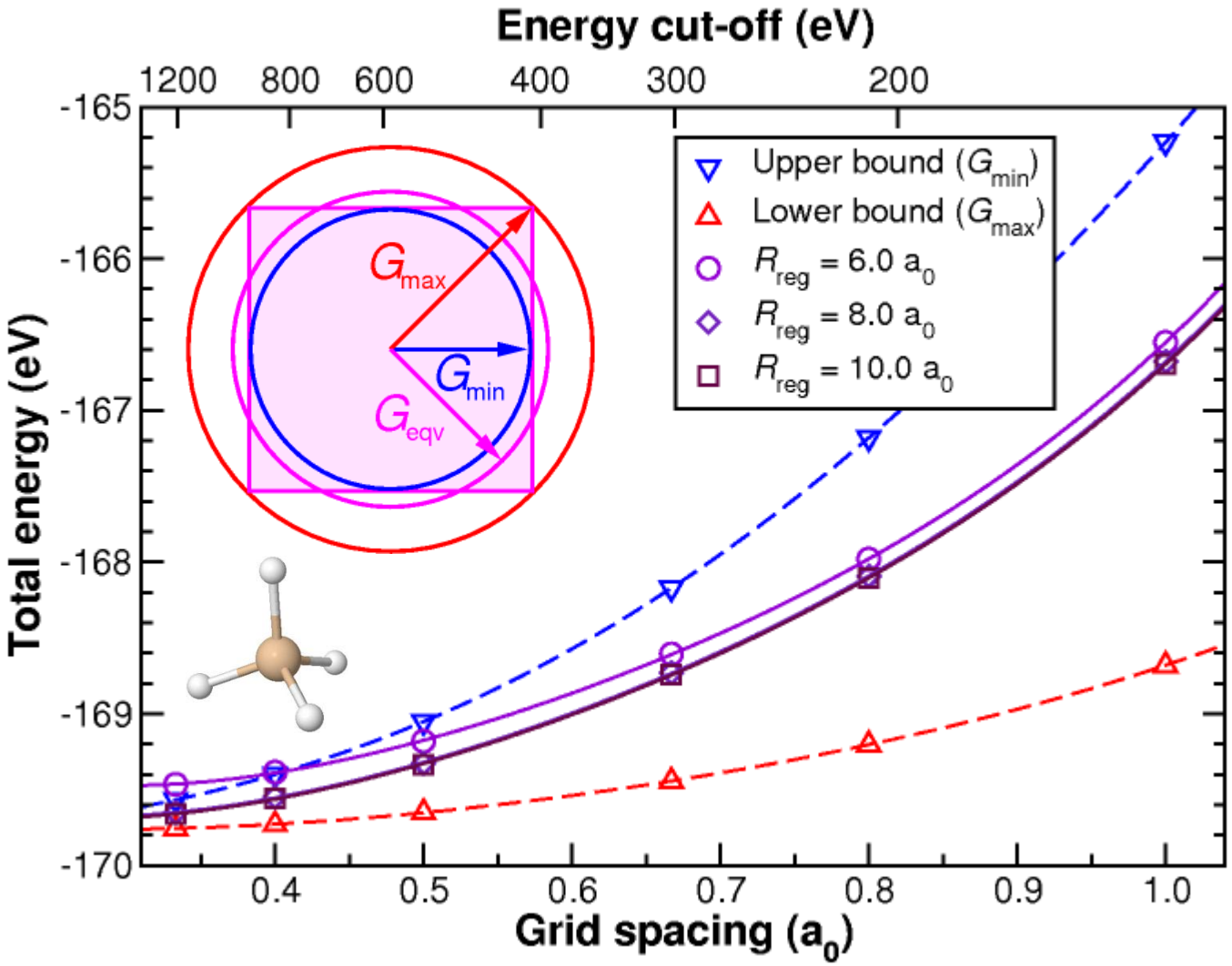




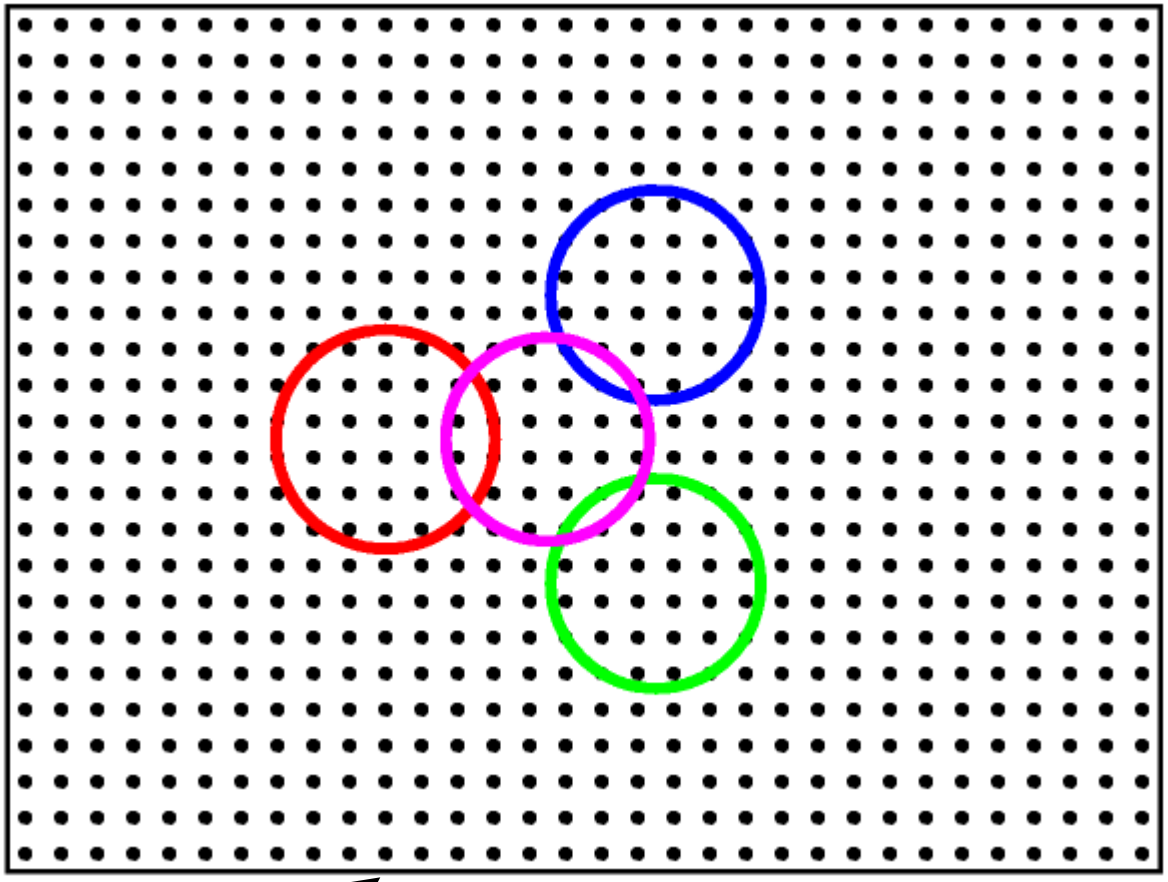
- Real linear combinations of plane-waves
- Localised
- Orthogonal

Mostofi, Haynes, Skylaris & Payne, *J. Chem. Phys.* **119**, 8842 (2003)

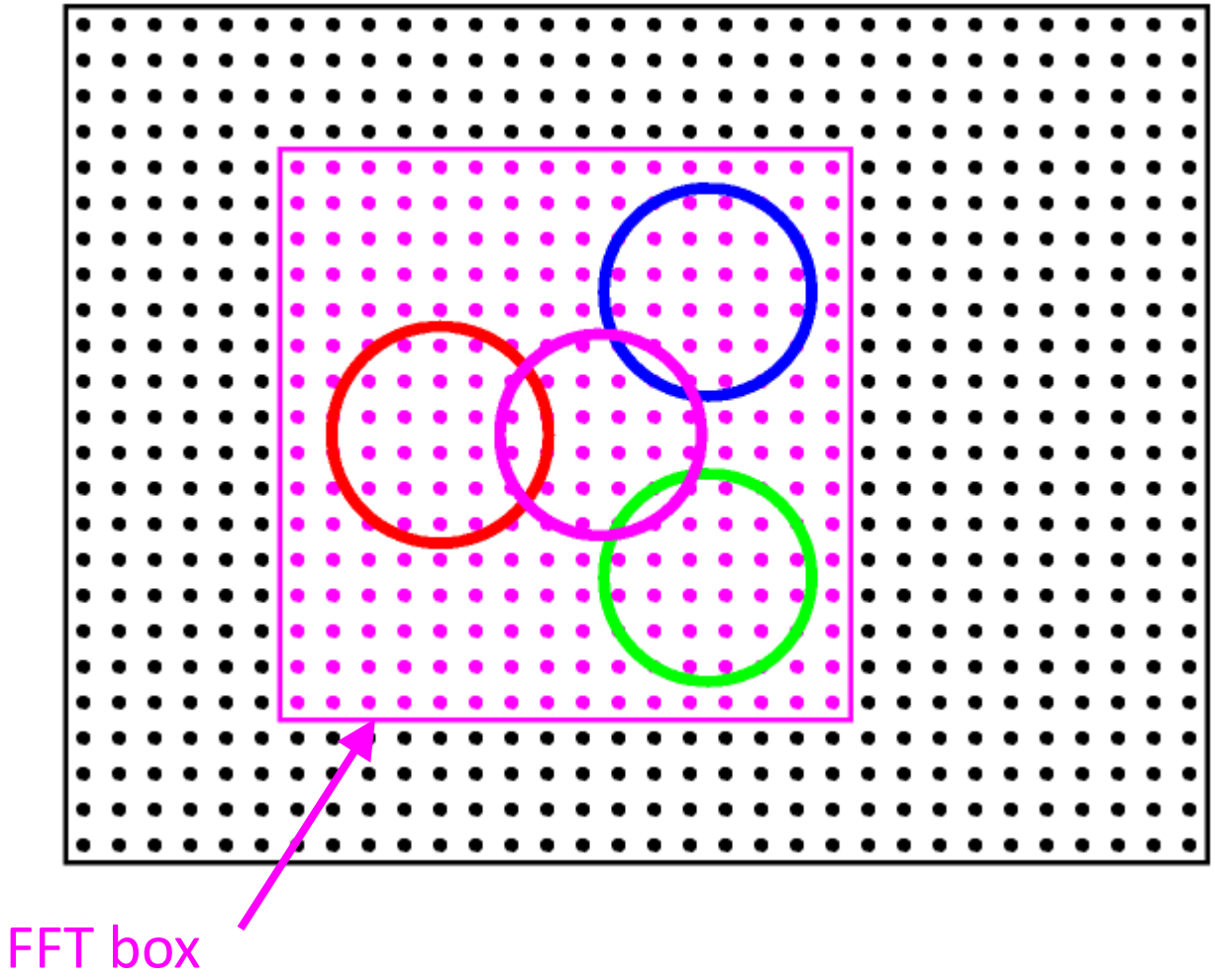
Psinc basis energy cut-off



FFT box technique

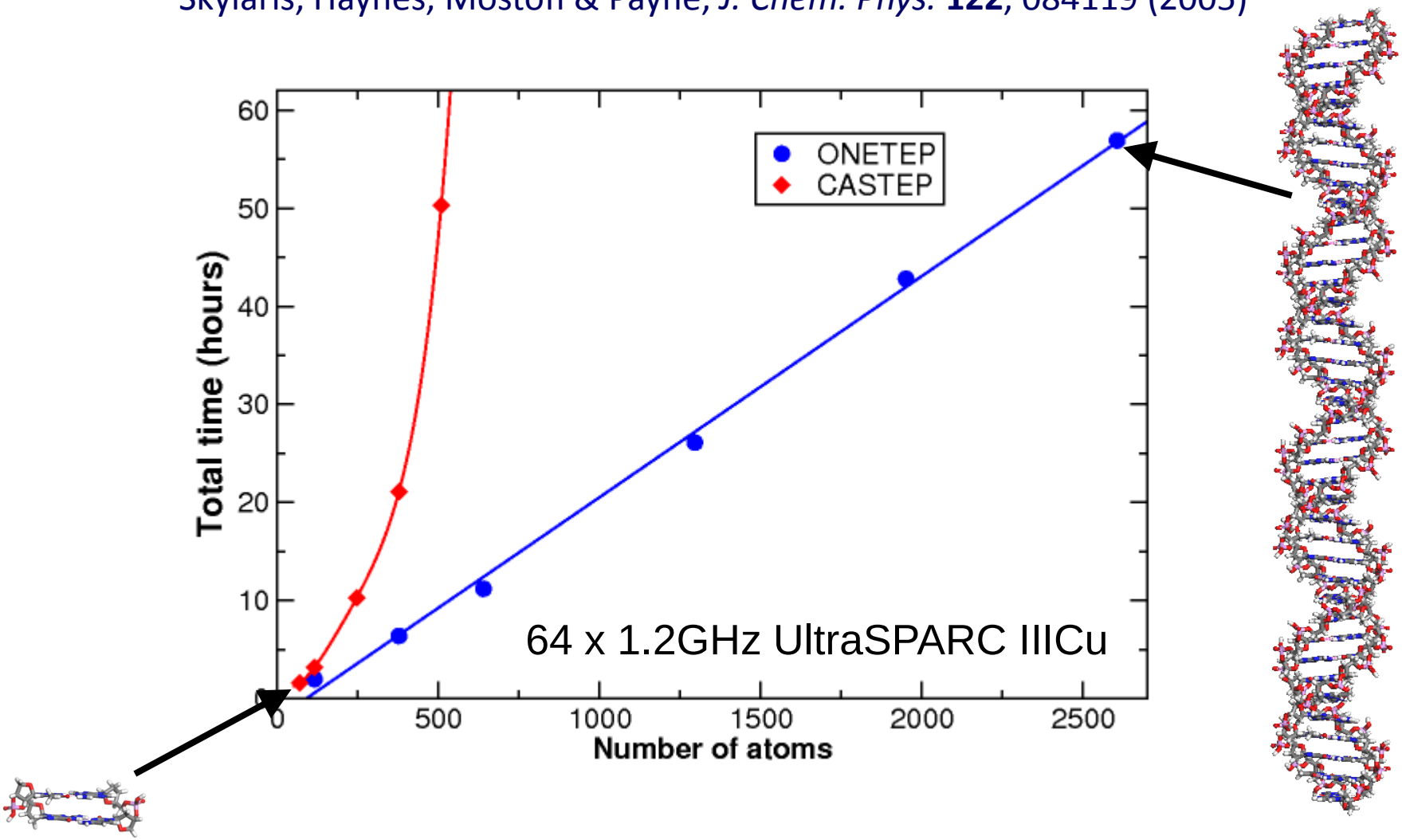


FFT box technique

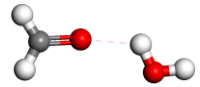


Linear scaling: DNA

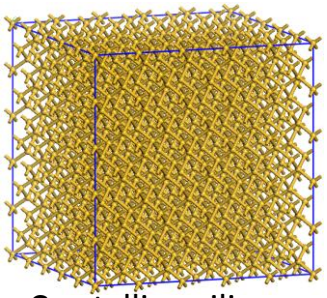
Skylaris, Haynes, Mostofi & Payne, *J. Chem. Phys.* **122**, 084119 (2005)



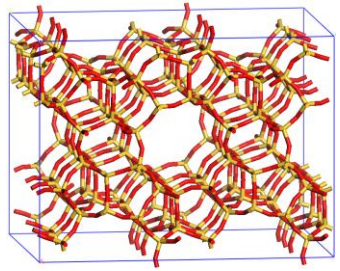
True linear scaling



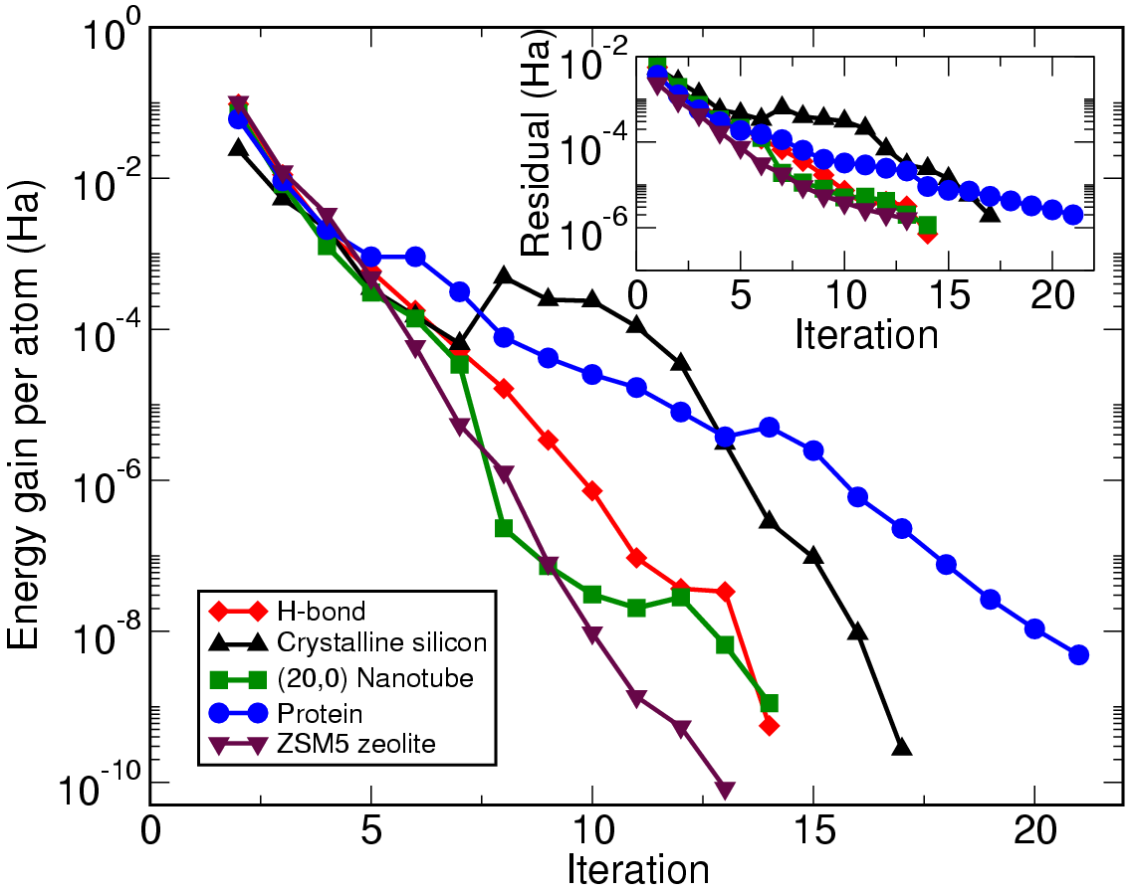
H-bond (7 atoms)

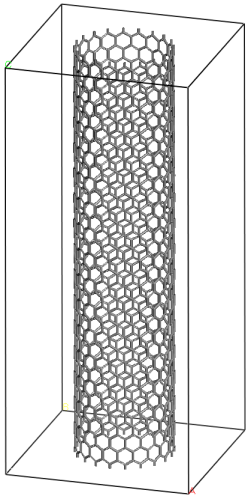


Crystalline silicon (1000 atoms)

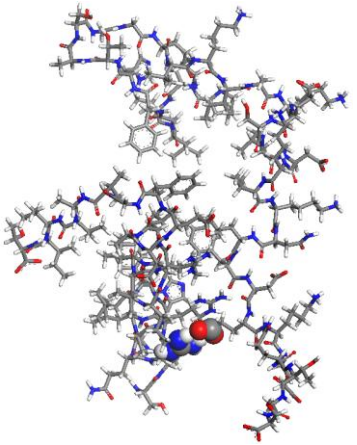


ZSM5 zeolite (576 atoms)





(20, 0) Nanotube (1280 atoms)



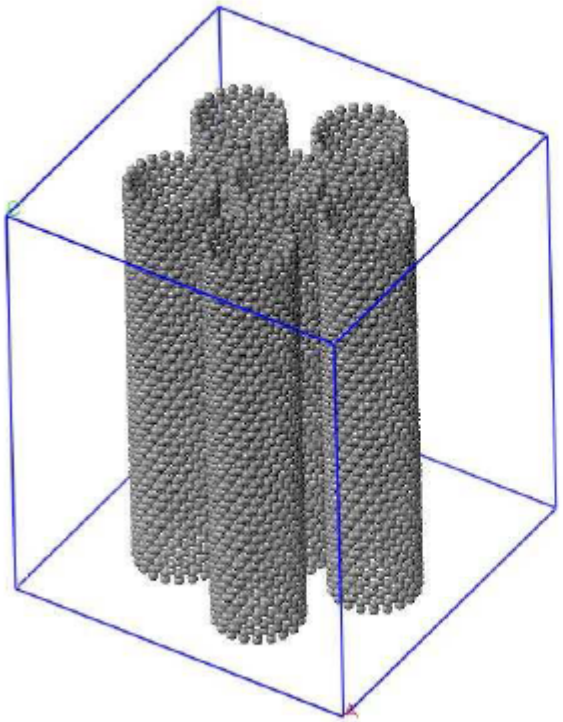
Protein (988 atoms)

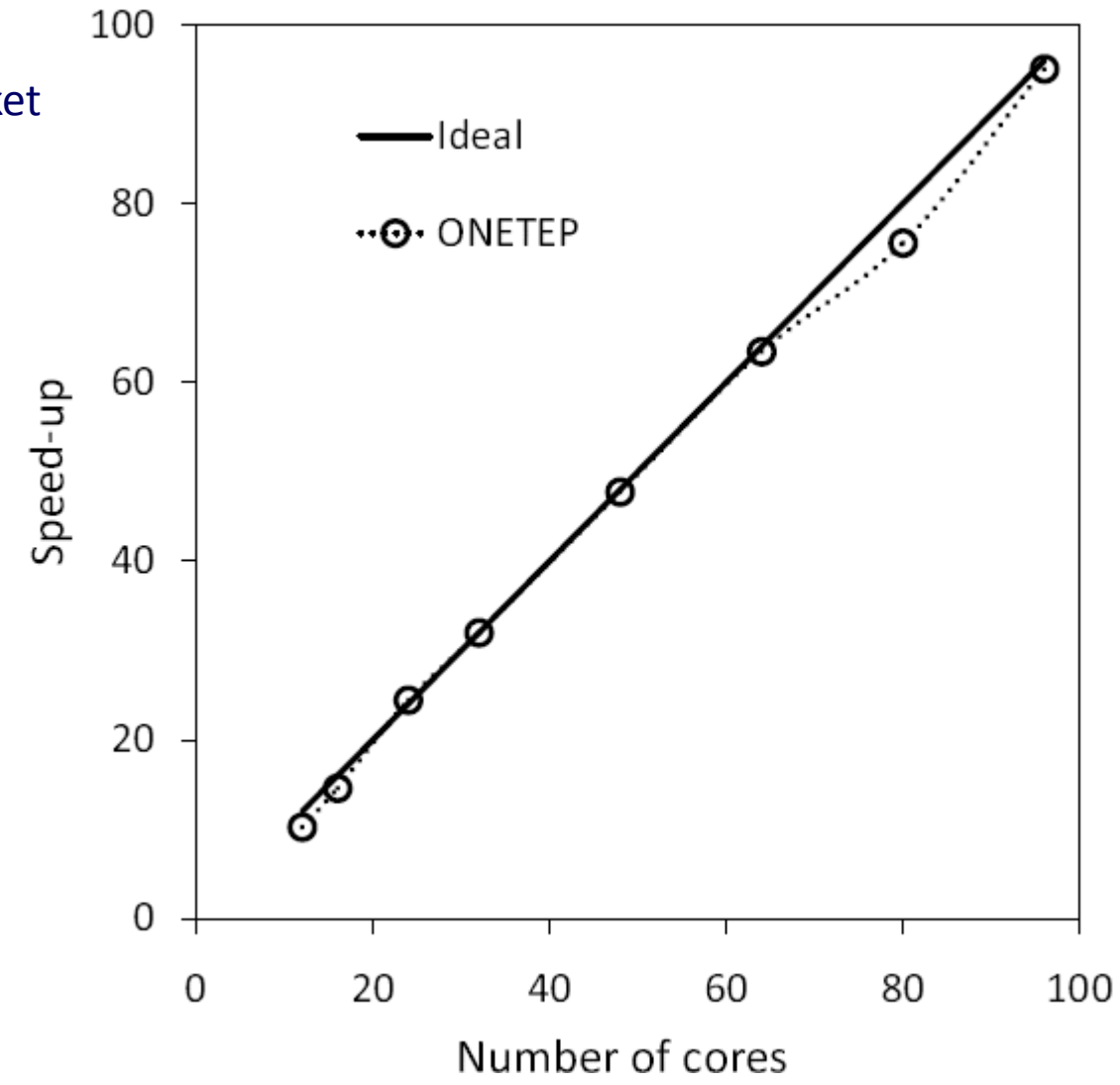
Skylaris, Haynes, Mostofi & Payne, *J. Phys.: Condens. Matter* **17**, 5757 (2005)

Parallel scaling: nanotubes

9600 atoms

Commodity cluster of 24 dual socket dual core Opteron nodes





Functionality

- LDA (Ceperley-Alder-Perdew-Zunger, Vosko-Wilk-Nusair) and GGA (Perdew-Wang ’91, Perdew-Burke-Ernzerhof & variants)
- Spin polarisation
- Forces
- Geometry optimisation
- Electronic structure analysis
- Visualisation
- Modified Coulomb interactions

Compiling ONETEP

- Simple multi-platform build system

- Fortran 90 compiler
- BLAS and LAPACK numerical libraries
- FFT library: vendor-supplied or FFTw
  - www.fftw.org
- MPI library for parallel version
  - www.lam-mpi.org

Running ONETEP

- Parallel computer
  - Minimum 1 GB per processor (core)
  - Typically distribute 100 atoms per processor
  - Cross-over >100 atoms

- Prepare input file: free format
  - Documentation at www.onetep.org

- Supply pseudopotential files (`.recpot` format)

Input file

- Keywords of different types:
  - Integer
  - Boolean
  - String
  - Real
  - Physical (real + unit)
  - Block data e.g. atomic positions, delimited by **`%block`** and **`%endblock`**
- Atomic units by default (hartree and bohr)
- Beware older keywords e.g. **`kernel_cutoff`**

Example input file: ethene

```
# Example input file
! Ethene molecule

cutoff_energy : 400 eV

%block  lattice_cart            ; in bohr
  40.000    0.000    0.000     ; a1
   0.000   40.000    0.000     ; a2
   0.000    0.000   40.000     ; a3
%endblock  lattice_cart

%block  species
H1  H  1  1  5.50     ; symbol, element, Z
C1  C  6  4  6.00     ; #NGWFs, radius (bohr)
%endblock  species
```

Example input file: ethene

```
%block  positions_abs   ; Cartesians, bohr
C1   21.231469   19.962216   20.048416
H1   22.316684   21.381117   21.086741
H1   22.305600   18.474510   19.097577
C1   18.768395   20.037541   19.951432
H1   17.694385   21.525477   20.902418
H1   17.683467   18.617139   18.913416
%endblock  positions_abs

%block  species_pot
H1   hydrogen.recpot
C1   carbon.recpot
%endblock  species_pot
```

ONETEP outline

- Initialisation phase:
  - Construct initial NGWFs (STOs or PAOs)
  - Construct initial charge density (atomic superposition) and effective potential
  - Construct initial Hamiltonian
  - Obtain initial (non-self-consistent) kernel using canonical purification
  - Refine initial kernel (self-consistently) using penalty functional

ONETEP outline continued

- Main optimisation phase:
  - Combination of nested self-consistent loops
  - Outer loop optimises the NGWFs (density kernel fixed)
  - Inner loop optimises the density kernel (NGWFs fixed)
- Final analysis phase:
  - Calculate forces
  - Write out potentials, densities, NGWFs for plotting
  - Mulliken population analysis
  - Diagonalisation yields wave functions, DOS etc.

Example output file: ethene

View ethene.out

More information

- www.onetep.org
- Scientific highlight of the month:
  - Ψ_k Newsletter **72**, December 2005
  - http://psi-k.dl.ac.uk/
- *J. Chem. Phys.* **122**, 084119 (2005)

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