Introduction to ONETEP

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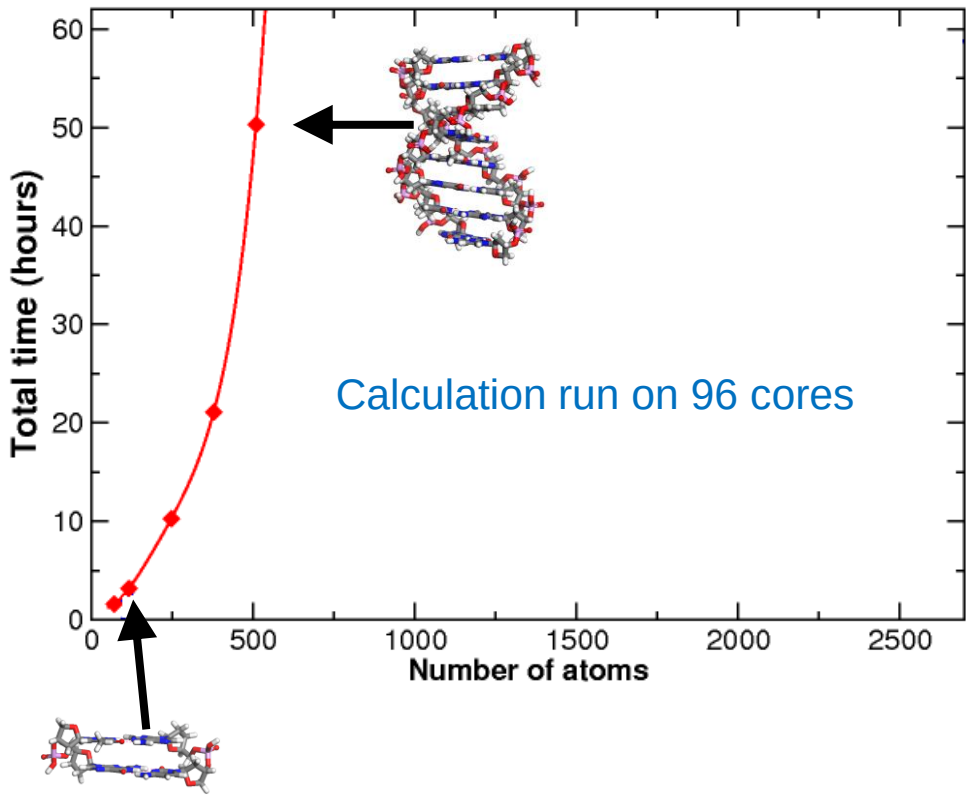
Outline

- Density matrix reformulation of DFT
- Localised function representation of density matrix
- Linear-scaling with localised functions
- Linear-scaling with large basis set accuracy
  - NGWFs, density kernel
  - Psinc basis set
  - FFT box
  - Linear-scaling examples
  - Parallel scaling
- Compilation and hardware requirements
- Running a simple calculation
- Functionality available

Computational cost of DFT: cubic-scaling



- Not a feasible approach for biomolecules with **thousands of atoms**
- A new, **linear-scaling reformulation of DFT,** is needed

Linear-scaling DFT based on the Density Matrix (DM)

- Physical principle

Nearsightedness of electronic matter
W. Kohn, *Phys. Rev. Lett*. **76**, 3168 (1996)

In molecules with non-zero band gap, the density matrix decays exponentially

$$\rho(\mathbf{r},\mathbf{r}') \sim e^{-\gamma|\mathbf{r}-\mathbf{r}'|} \to 0 \quad \text{as} \quad |\mathbf{r}-\mathbf{r}'| \to \infty$$

- Linear-scaling approaches

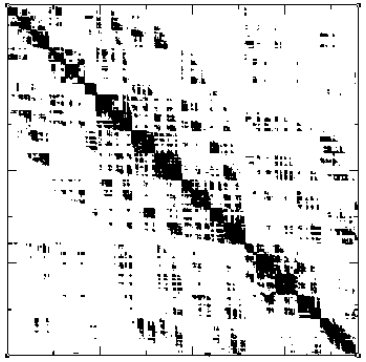
Truncate exponential "tail"

$$\rho(\mathbf{r},\mathbf{r}') = 0 \quad \text{when} \quad |\mathbf{r}-\mathbf{r}'| > r_{\text{cut}}$$

- Practical implementation

Localised functions, sparse matrix algebra

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



DFT with the one-particle Density Matrix instead of Molecular Orbitals

Density matrix

$$\rho(\mathbf{r},\mathbf{r}') = \sum_i f_i\, \psi_i(\mathbf{r})\, \psi_i^*(\mathbf{r}')$$

Density

$$n(\mathbf{r}) = \sum_i |\psi_i(\mathbf{r})|^2$$

$$n(\mathbf{r}) = \rho(\mathbf{r},\mathbf{r})$$

Energy expressions

With molecular orbitals

$$E[\{\psi_j\}] = \sum_i \int \psi_i(\mathbf{r}) \left(-\frac{1}{2}\nabla^2\right) \psi_i(\mathbf{r})\, d\mathbf{r} + \int V_{\text{ext}}(\mathbf{r}) n(\mathbf{r})\, d\mathbf{r} + \frac{1}{2}\int\int \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}\, d\mathbf{r}' + E_{xc}[n]$$

With density matrix

$$E[\rho] = \int \left[-\frac{1}{2}\nabla^2_{\mathbf{r}'}\rho(\mathbf{r}',\mathbf{r})\right]_{\mathbf{r}'=\mathbf{r}} d\mathbf{r} + \int V_{\text{ext}}(\mathbf{r}) n(\mathbf{r})\, d\mathbf{r} + \frac{1}{2}\int\int \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\, d\mathbf{r}\, d\mathbf{r}' + E_{xc}[n]$$

One-particle density matrix

Operator representation

$$\hat{\rho} = \sum_n f_n |\psi_n\rangle\langle\psi_n|$$

Position representation

$$\langle \mathbf{r}|\hat{\rho}|\mathbf{r}'\rangle = \rho(\mathbf{r},\mathbf{r}') = \sum_n f_n\, \psi_n(\mathbf{r})\psi_n^*(\mathbf{r}')$$

Conditions

- **Idempotency** (from **orbital orthonormality and occupancies 1 or 0**)

$$\rho^2(\mathbf{r},\mathbf{r}') = \int \rho(\mathbf{r},\mathbf{r}'')\rho(\mathbf{r}'',\mathbf{r}')d\mathbf{r}'' = \sum_n f_n^2 \psi_n(\mathbf{r})\psi_n^*(\mathbf{r}') = \sum_n f_n \psi_n(\mathbf{r})\psi_n^*(\mathbf{r}') = \rho(\mathbf{r},\mathbf{r}')$$

- **Normalisation** (preserving the **number of electrons**)

$$\mathrm{tr}[\rho] = \int \rho(\mathbf{r},\mathbf{r})d\mathbf{r} = \int \sum_n f_n\, \psi_n(\mathbf{r})\psi_n^*(\mathbf{r})\, d\mathbf{r} = \sum_n f_n \int |\psi_n(\mathbf{r})|^2 d\mathbf{r} = \sum_n f_n = N_e$$

Linear-scaling DFT: Density matrix in localised functions

$$\psi_n(\mathbf{r}) = \phi_\alpha(\mathbf{r}) M^\alpha_{\ n}$$

Molecular Orbital (MO)

Atomic Orbital (AO)

Overlap matrix

$$S_{\alpha\beta} = \langle \phi_\alpha | \phi_\beta \rangle$$

$$\rho(\mathbf{r},\mathbf{r}') = \sum_n f_n \psi_n(\mathbf{r}) \psi_n^*(\mathbf{r}') = \phi_\alpha(\mathbf{r}) \left(\sum_n M^\alpha_{\ n} f_n M_n^{\dagger\,\beta} \right) \phi_\beta^*(\mathbf{r}') = \boxed{\phi_\alpha(\mathbf{r}) K^{\alpha\beta} \phi_\beta^*(\mathbf{r}')}$$

Conditions

- **Idempotency**

$$\mathbf{KSK} = \mathbf{K}$$

- **Normalisation**

$$\mathrm{tr}[\rho] = \mathrm{tr}[\mathbf{KS}] = N_e$$

$$K^{\alpha\beta} = \sum_n M^\alpha_{\ n} f_n M_n^{\dagger\,\beta}$$

Density kernel

Linear-scaling DFT in practice

Conflicting requirements

- Localised functions
- Sparse matrices

Large basis set accuracy

Linear-scaling cost

- Delocalised functions
- Dense matrices

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

Linear-scaling cost with “cubic-scaling accuracy”

Two levels of resolution

- Coarse
  - **Minimal set of localised non-orthogonal functions**
- Fine
  - **Large, near-complete basis set**
  - ***In situ* optimisation of the minimal set of non-orthogonal functions**

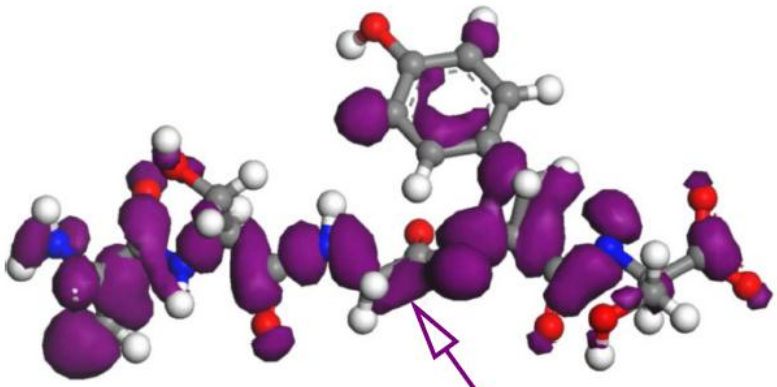
Optimal basis density matrix minimization (OBDMM) approaches

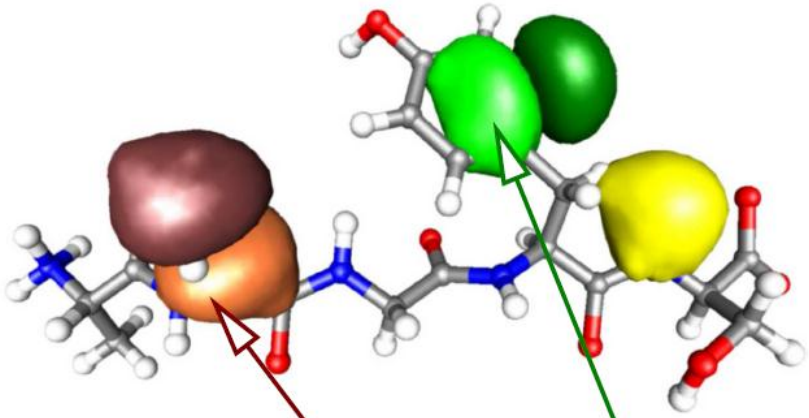
(S. Goedecker, *Rev. Mod. Phys.*, **71**, 1085 (1999))

E. Hernandez and M. J. Gillan, *Phys. Rev. B* **51**, 10157 (1995).
J.-L. Fattebert and J. Bernholc, *Phys. Rev. B* **62**, 1713 (2000).
C.-K. Skylaris, A. A. Mostofi, P. D. Haynes, O. Dieguez and M. C. Payne, *Phys. Rev. B* **66**, 035119 (2002).

The ONETEP approach

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





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

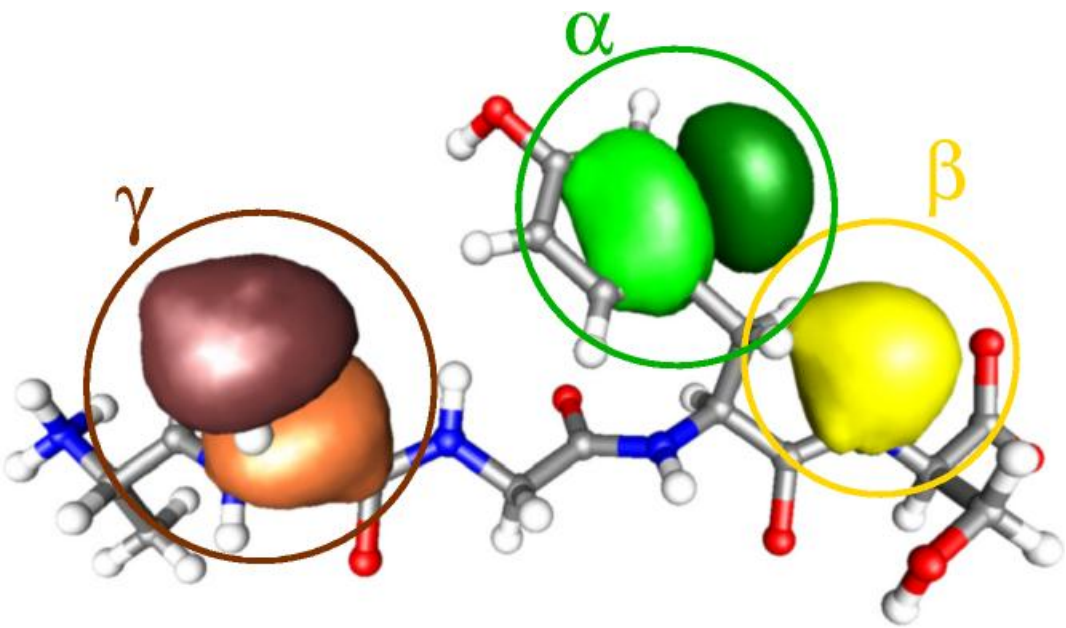
Molecular orbitals (MOs)

Non-orthogonal Generalised Wannier Functions (NGWFs)

Density kernel

- Coarse level: The NGWFs are the localised orbitals
- Fine level: NGWFs expanded in a basis set of psinc functions

Density matrix localisation



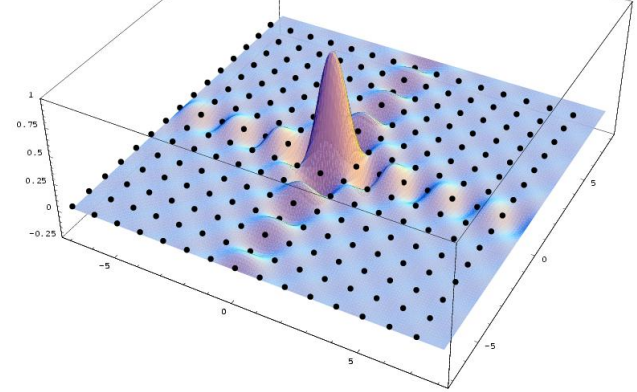
$$\rho(\mathbf{r},\mathbf{r}') = \sum_{\alpha\beta} \phi_\alpha(\mathbf{r}) K^{\alpha\beta} \phi_\beta(\mathbf{r}')$$

- Impose spatial cut-offs:
  - NGWFs confined to spherical regions
  - Sparse density kernel $\boldsymbol{K}$ by truncation

Basis set: Psinc functions

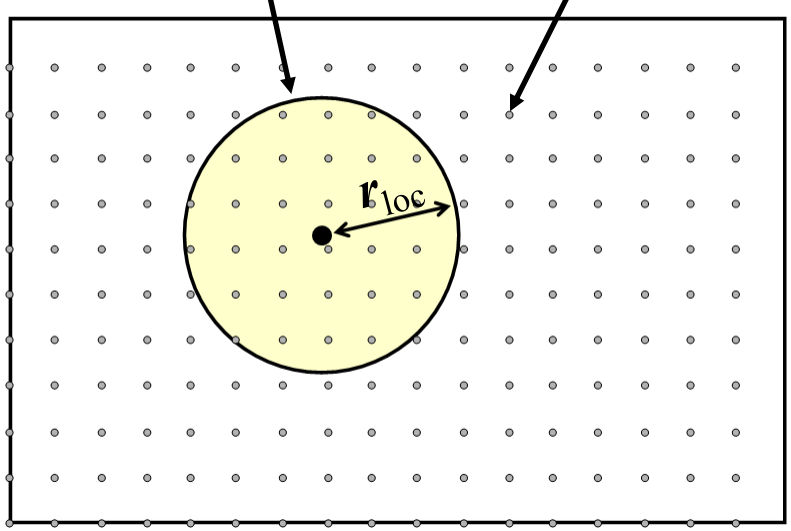
- Real linear combinations of plane waves $$D_j(\mathbf{r}) = \frac{1}{N}\sum_{\mathbf{G}}^{\mathbf{G}_{\max}} e^{i\mathbf{G}\cdot(\mathbf{r}-\mathbf{r}_j)}$$
- Highly localised
- Orthogonal

in 2D: $D_j(\mathbf{r}) = D_j(x)D_j(y)D_j(z)$



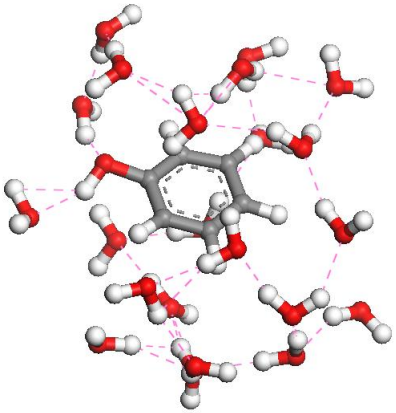
NGWF localisation sphere

$\mathbf{r}_i$ centre of $D_i(\mathbf{r})$



- A. A. Mostofi, P. D. Haynes, C.-K. Skylaris and M. C. Payne, *J. Chem. Phys.* **119**, 8842 (2003)
- D. Baye and P. H. Heenen, *J. Phys. A: Math. Gen.* **19**, 2041 (1986)

Near-complete basis set accuracy



Binding energy calculation

ONETEP (psinc basis set, K.E. cutoff 800eV)

NGWF radii (Å)	# NGWFs	BE (kcal/mol)
2.9	166	**-11.93**
3.2	166	**-12.86**
3.7	166	**-8.25**
4.2	166	**-7.06**
4.8	166	**-7.04**

ONETEP is basis set variational

C.-K. Skylaris, O. Dieguez, P. D. Haynes and M. C. Payne, *Phys. Rev. B* **66**, 073103 (2002).

NWChem (Gaussian basis set, including BSSE correction)

Basis set	# AOs	BE (kcal/mol)	BE + BSSE (kcal/mol)
STO-3G	195	-23.17	**-7.98**
3-21G	361	-46.48	**-12.55**
6-31G*	535	-27.77	**-8.95**
6-311+G*	817	-17.71	**-8.79**
6-311++G**	1017	-12.49	**-7.39**
cc-pVDZ	685	-33.26	**-7.28**
cc-pVTZ	1765	-19.59	**-7.04**
cc-PVQZ	3780	-12.41	**-7.22**

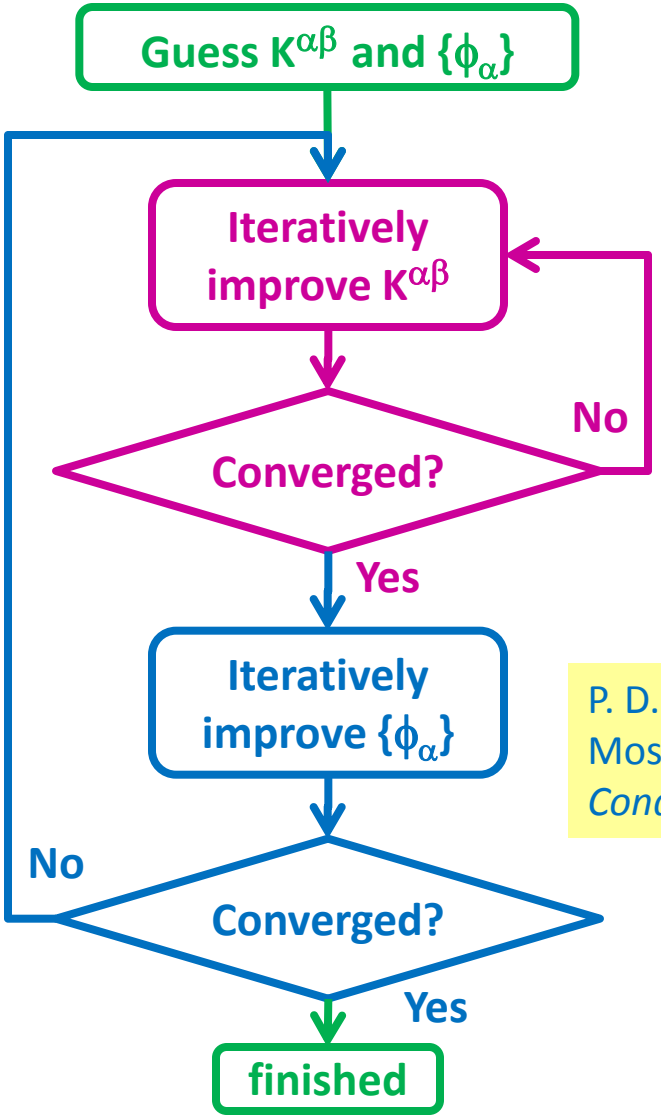
No B.S.S.E. correction needed with psinc basis

P. D. Haynes, C.-K. Skylaris, A. A. Mostofi and M. C. Payne, *Chem. Phys. Lett.* **422** 345 (2006).

Energy optimisation in ONETEP

$$E = E[\mathbf{K}, \{\phi_\alpha\}]$$

- **Outer loop:** Optimise total (interacting) energy *E* w.r.t. to **K and** $\{\phi_\alpha\}$

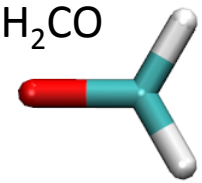


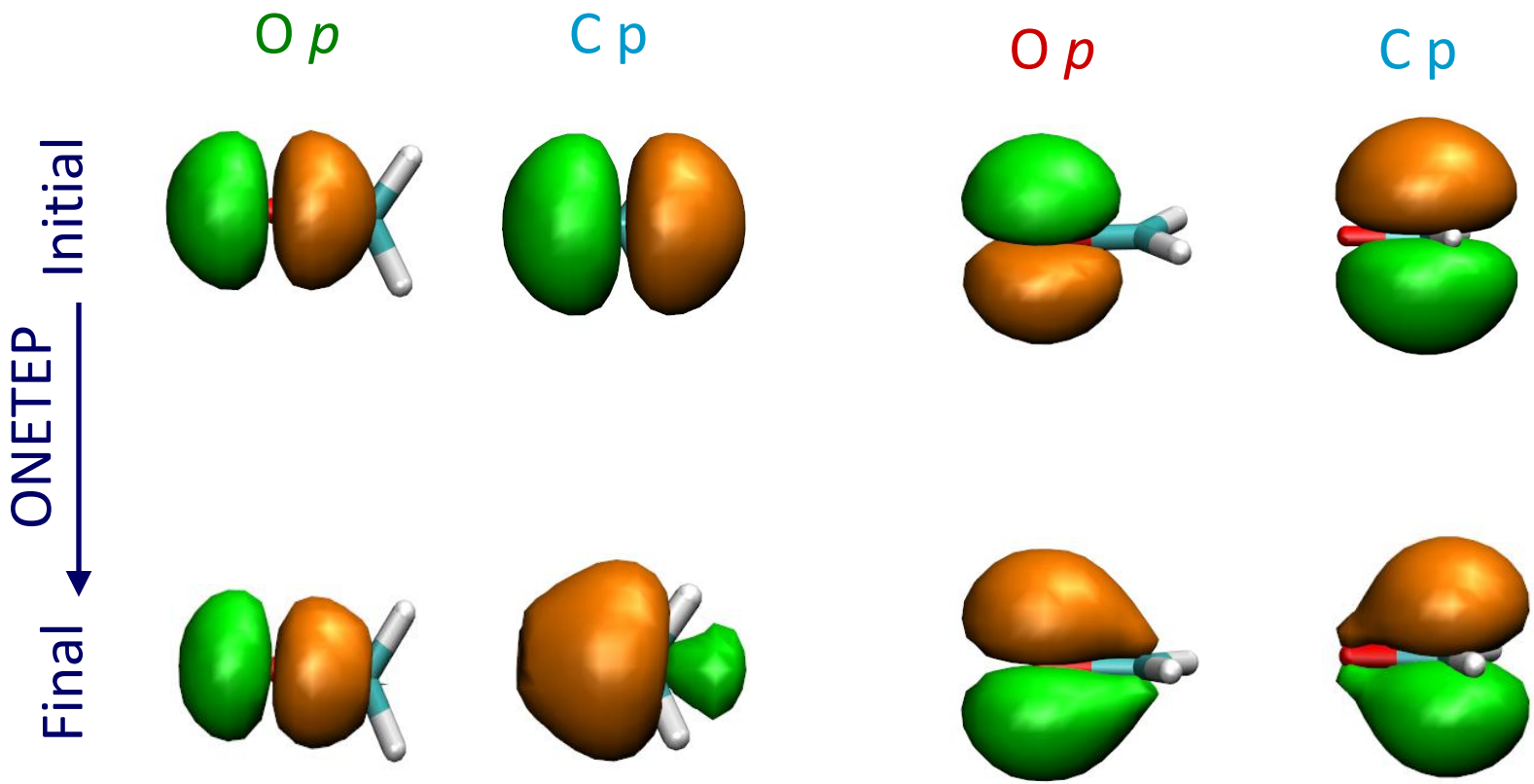
- **Inner loop**: Optimise total (interacting) energy *E* w.r.t **K** for fixed $\{\phi_\alpha\}$ while imposing **idempotency** and **normalisation**

P. D. Haynes, C.-K. Skylaris, A. A. Mostofi and M. C. Payne, *J. Phys. Condens*. Matter **20**, 294207 (2008)

NGWF optimisation

formaldehyde, H_2CO





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NGWF optimisation

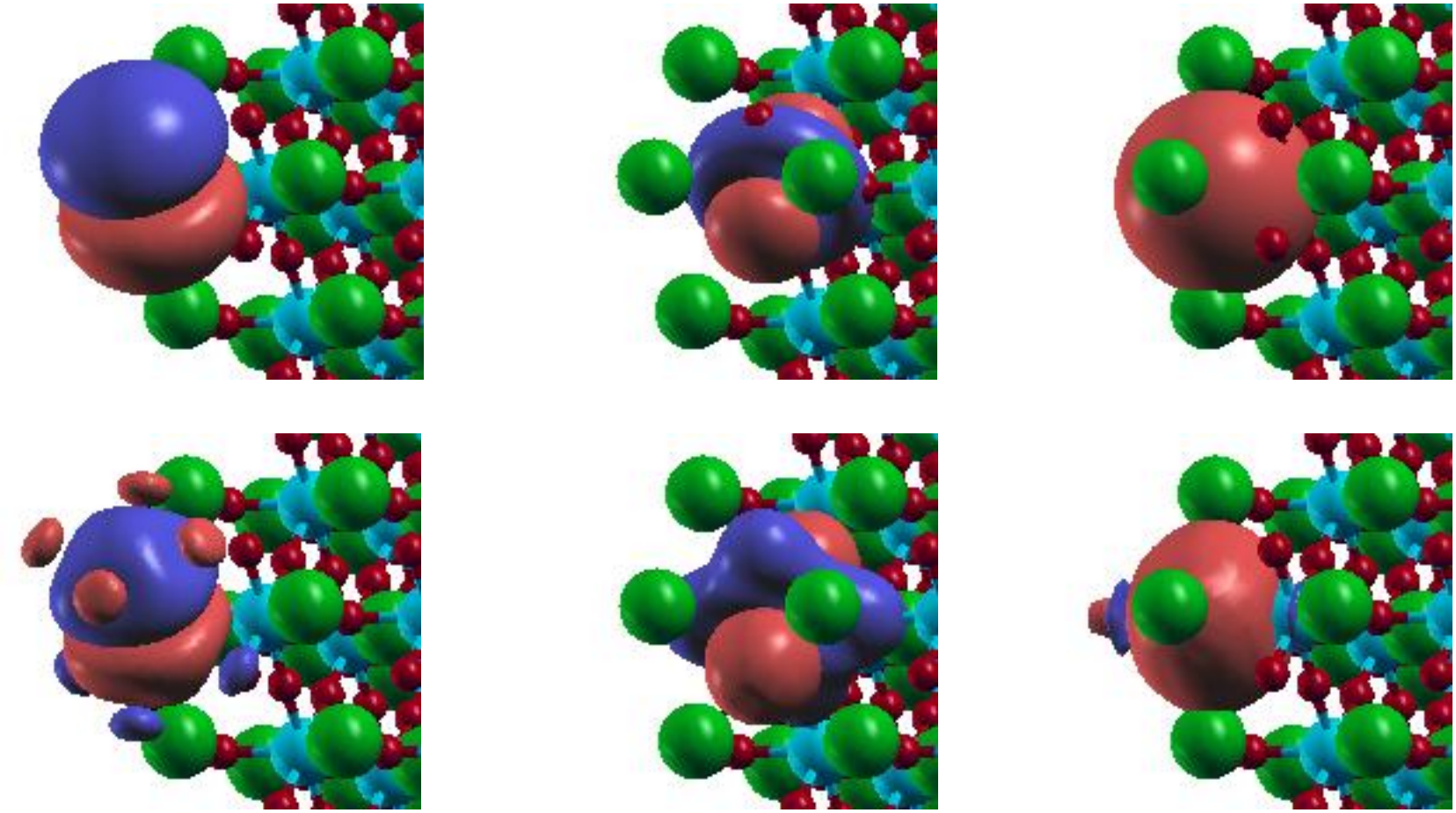
$BaTiO_3$

Ba *p* | Ti *d* | O *s*

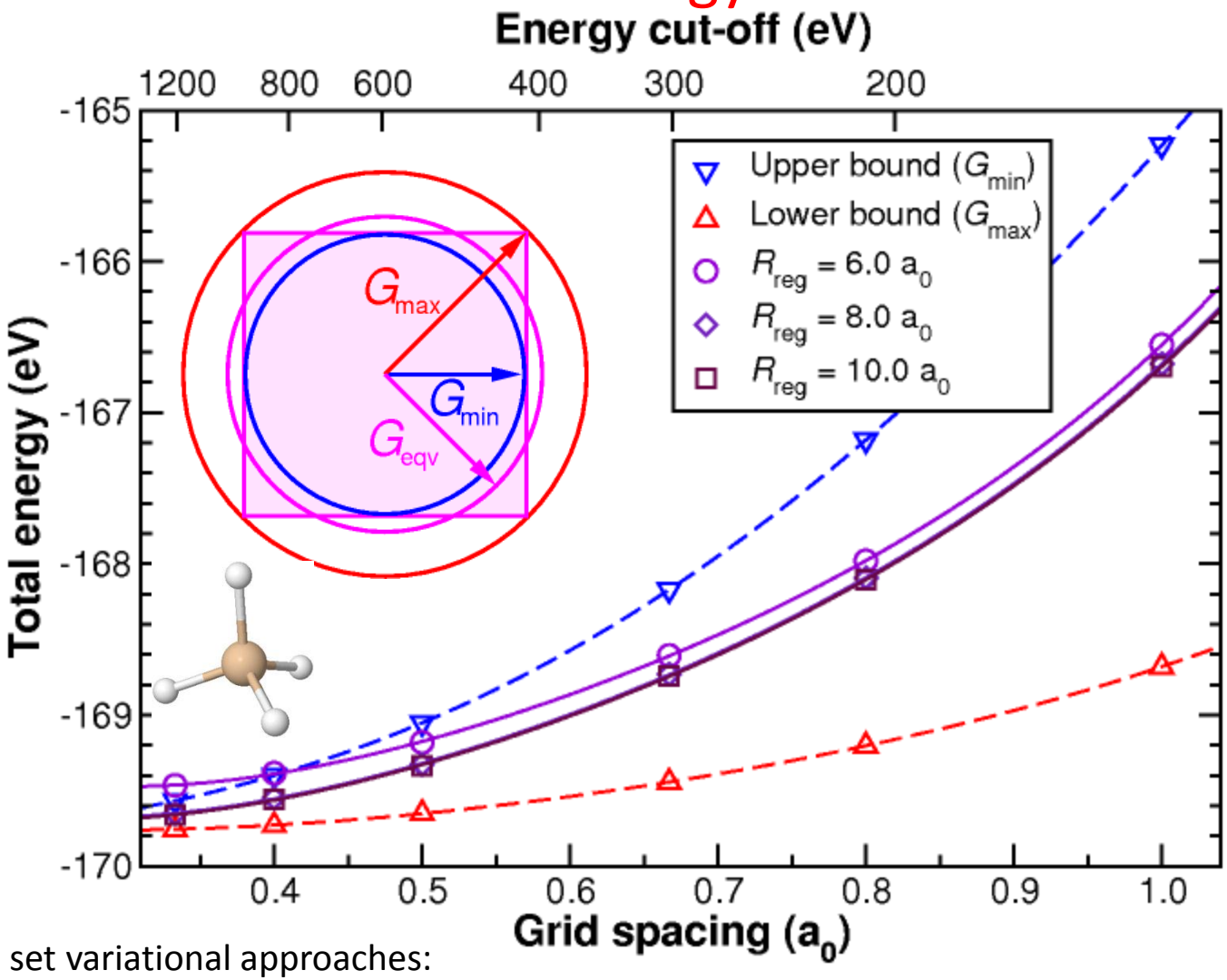
Initial

ONETEP

Final



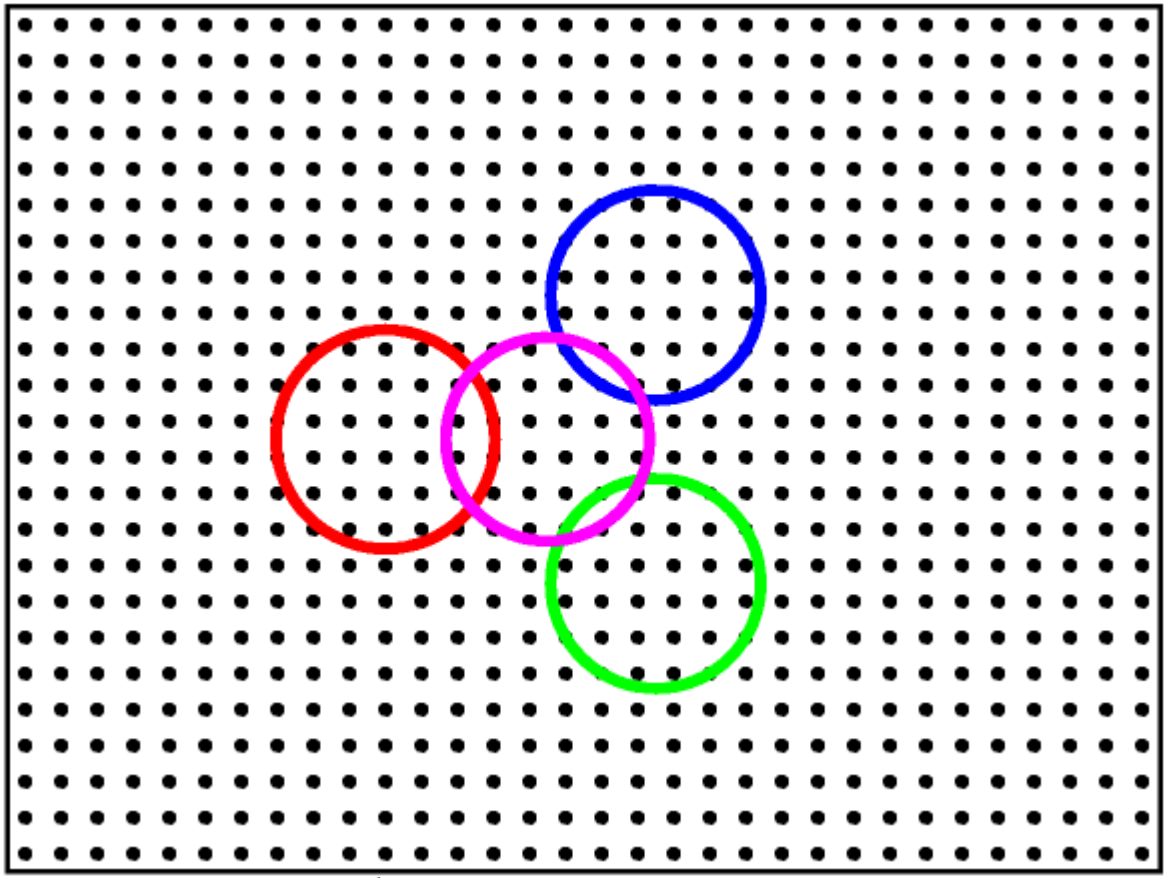
Psinc basis energy cut-off



Basis set variational approaches:

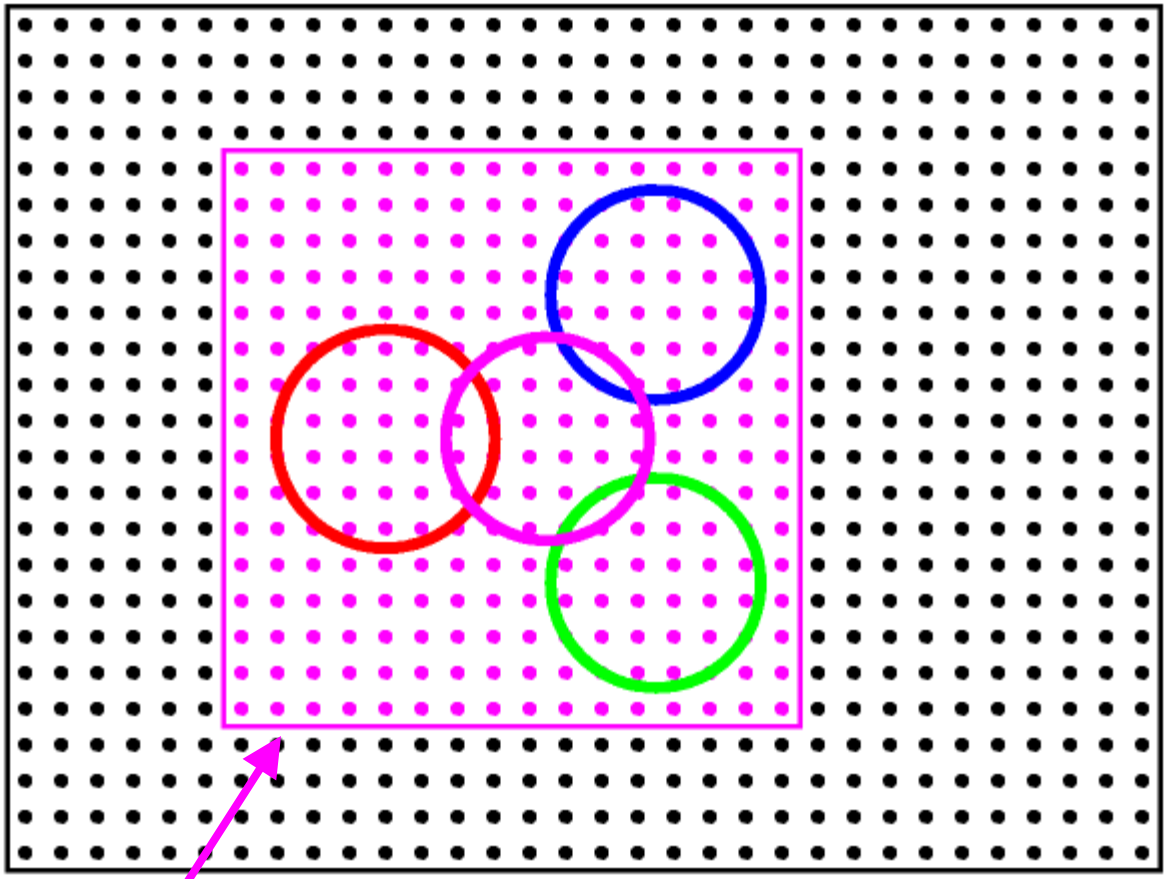
C.-K. Skylaris, O. Dieguez, P. Haynes and M. C. Payne, *Phys. Rev. B* **66**, 073103 (2002).

FFT box technique



simulation cell

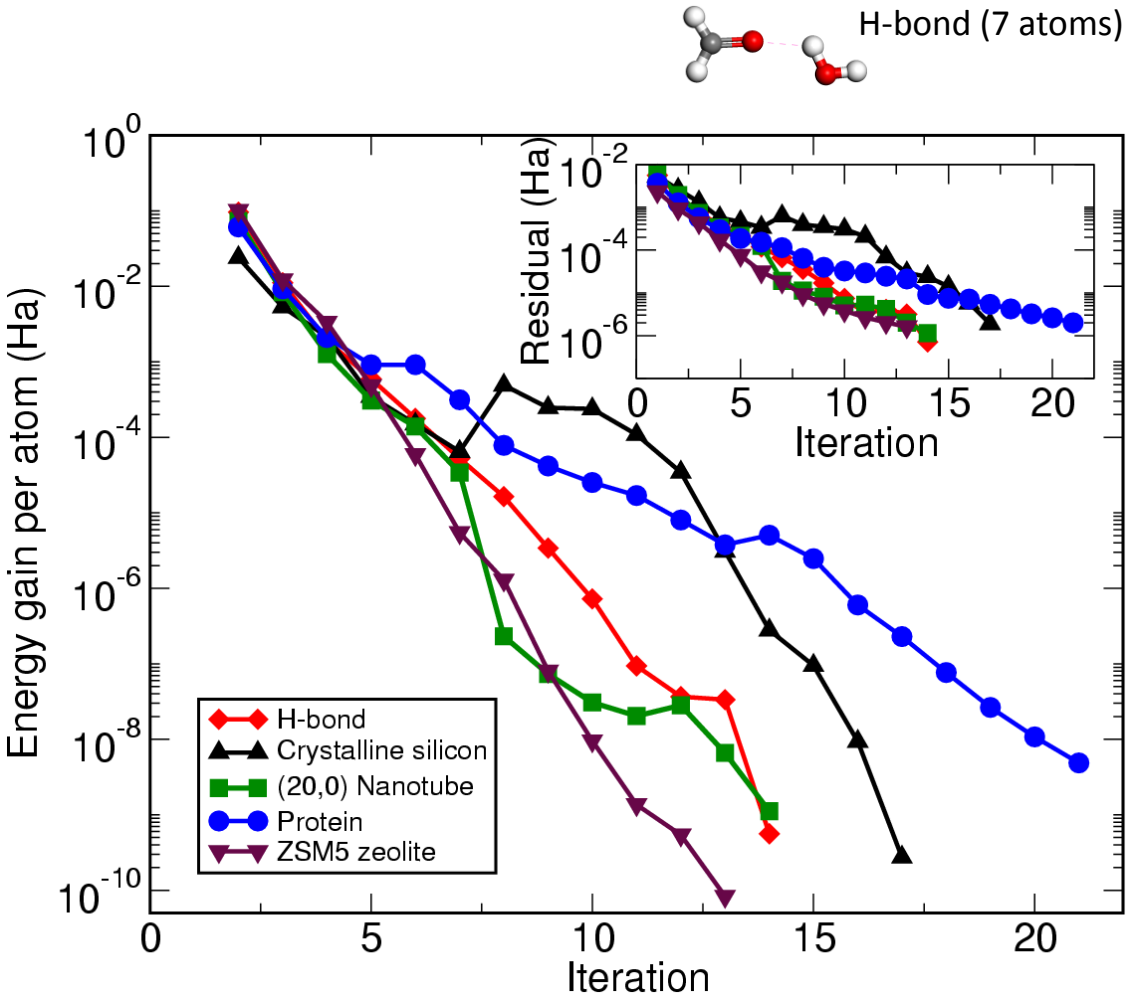
FFT box technique

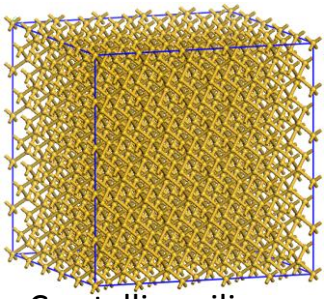


FFT box

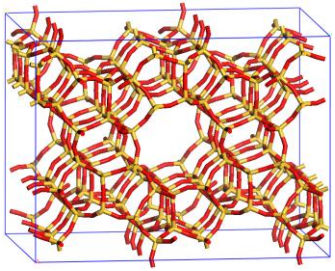
C.-K. Skylaris, A. A. Mostofi, P. D. Haynes, C. J. Pickard & M. C. Payne, *Comp. Phys. Comm.* **140**, 315 (2001)
A. A. Mostofi, C.-K. Skylaris, P. D. Haynes & M. C. Payne, *Comp. Phys. Comm.* **147**, 788 (2002)

True linear scaling

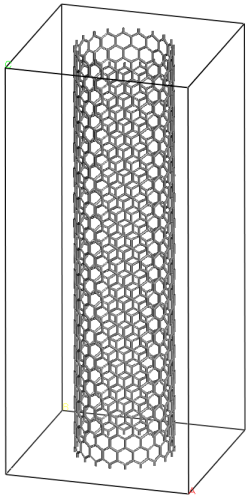




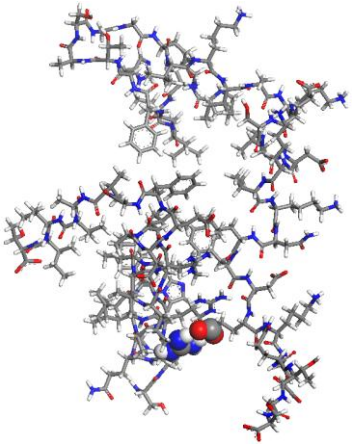
Crystalline silicon (1000 atoms)



ZSM5 zeolite (576 atoms)



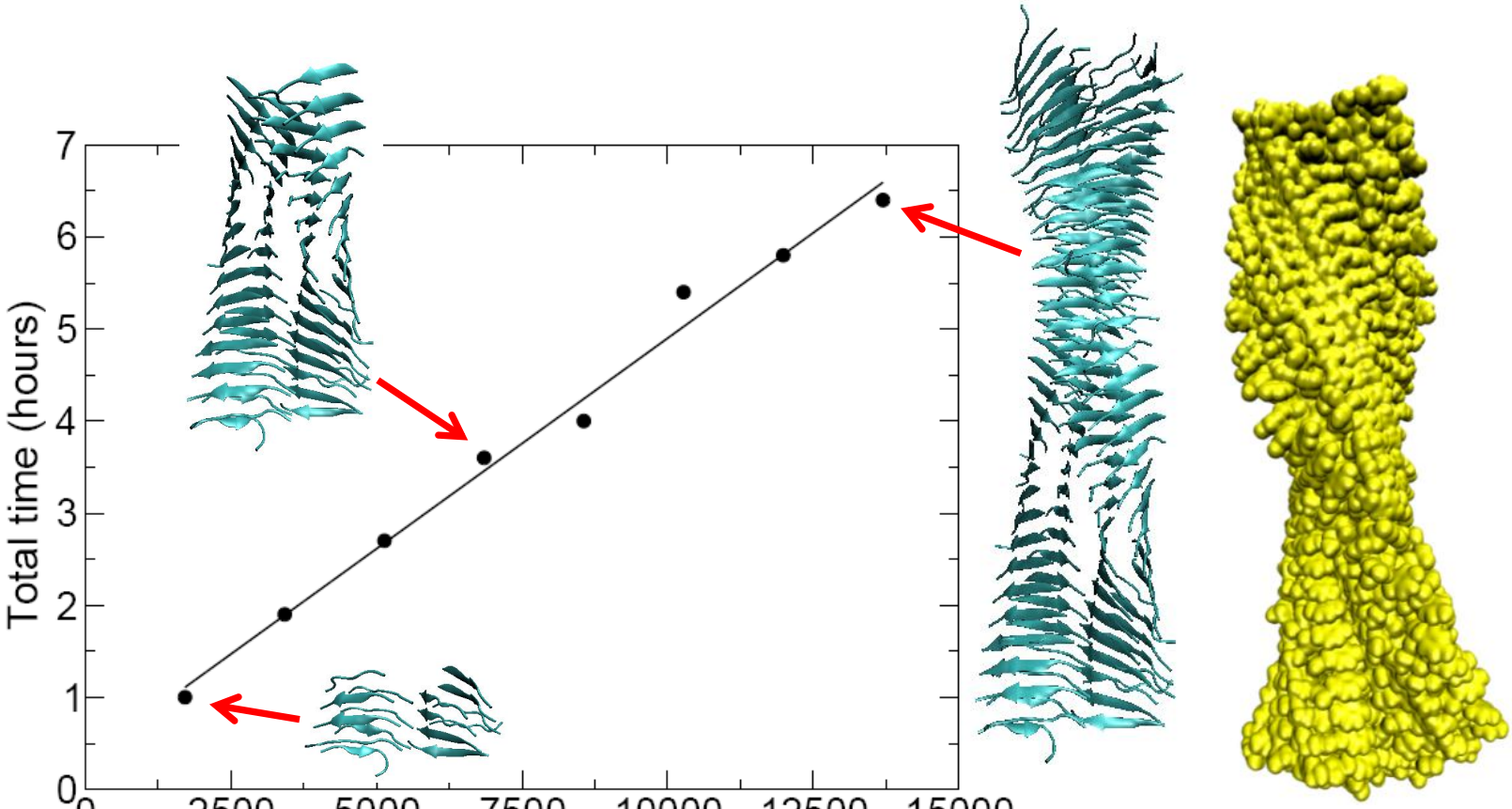
(20, 0) Nanotube (1280 atoms)



Protein (988 atoms)

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

Linear-scaling: Amyloid fibrils



Electronic density from ONETEP calculation

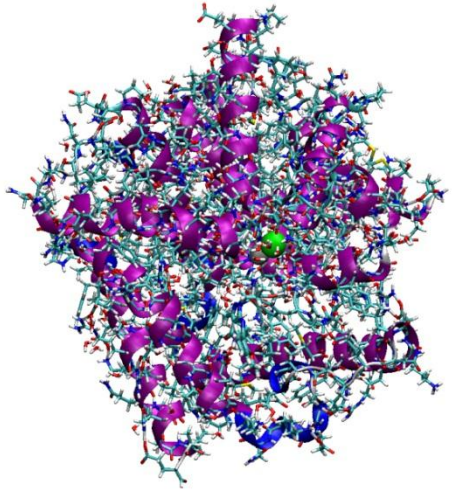
Structures of the amyloid fibril kindly provided by the authors of
*J. T. Berryman, S. E. Radford and S. A. Harris, Biophysical Journal, **97** 1 (2009)*

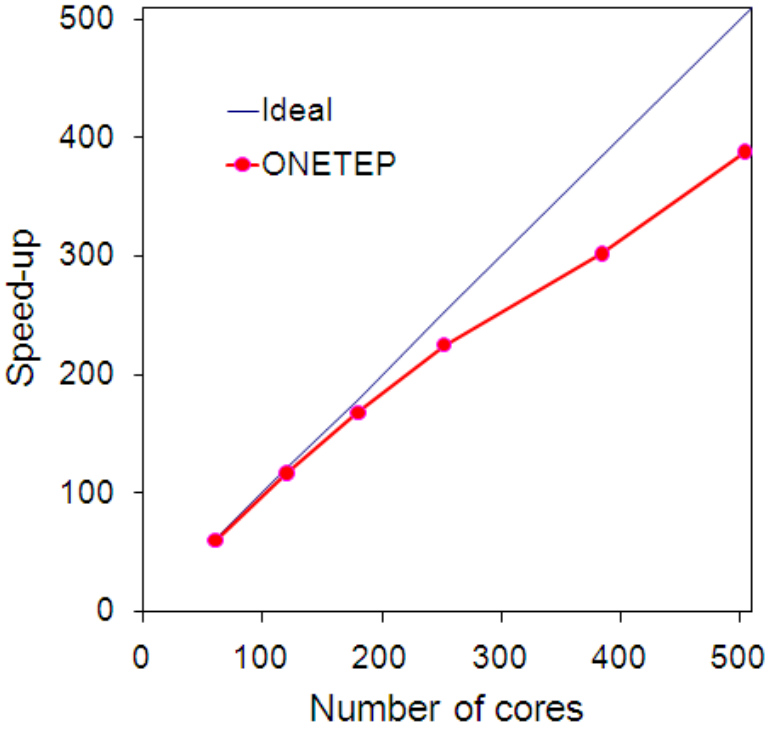
Parallel implementation

- Message Passing Interface (MPI), Fortran 2003 and standard mathematical libraries

Skylaris, Haynes, Mostofi & Payne, *Phys. Stat. Sol. (b)* **243**, 973 (2006)
Hine, Haynes, Mostofi, Skylaris & Payne, *Comput. Phys. Comm.* **180**, 1041 (2009)

- Example: Speed-up for PDE5 protein (5756 atoms)





- Porting on GPU cards

K. Wilkinson and C.-K. Skylaris, *J Comp. Chem.* **Accepted for publication** (2013)

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Compiling ONETEP

Simple multi-platform build system, needs:

- Fortran 2003 compiler
- BLAS and LAPACK (or SCALAPACK) numerical libraries
- FFT library: vendor-supplied or FFTw
  - www.fftw.org
- MPI library for parallel version

Running ONETEP

- Parallel computer
  - Minimum 2 GB per processor (core)
  - Typically distribute 10-100 atoms per processor
  - Cross-over >100 atoms

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

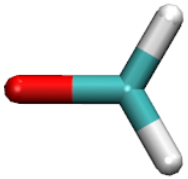
- Supply pseudopotential files (`.recpot` format)

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)

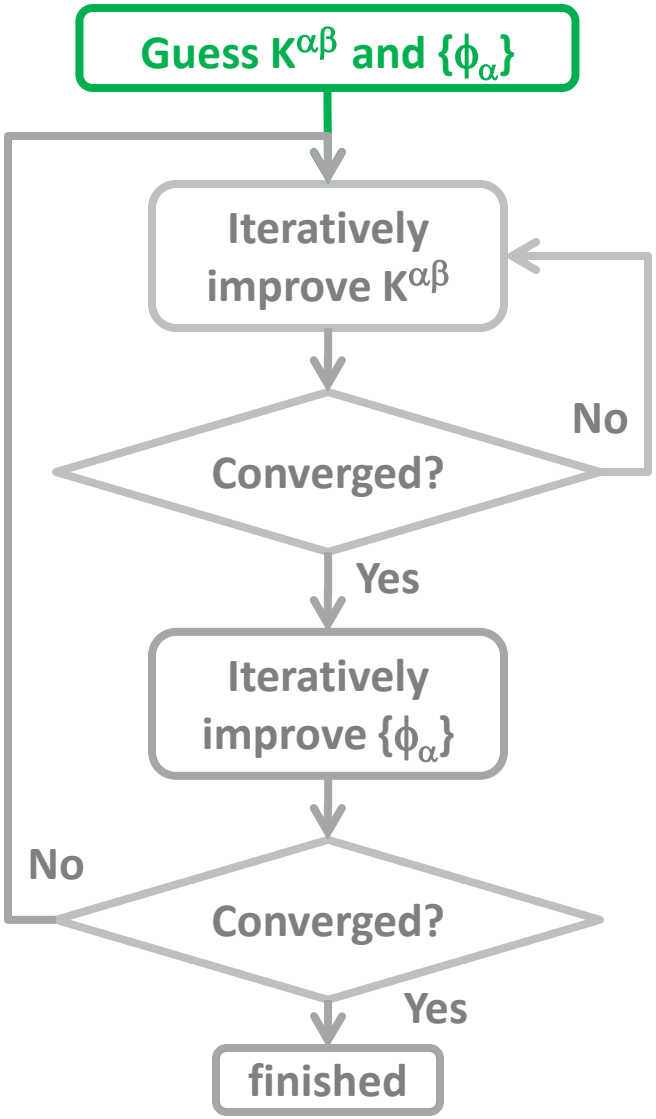
Example input file: formaldehyde

```
! Example input file for the ONETEP program
! Formaldehyde molecule

cutoff_energy 600 eV

%block   lattice_cart
  48.00      0.00      0.00
   0.00     48.00      0.00
   0.00      0.00     48.00
%endblock  lattice_cart

%block  positions_abs
O      24.887507   23.896975   22.647313
C      27.731659   23.667449   22.643306
H      28.655157   21.721170   22.637547
H      28.955467   25.440371   22.646039
%endblock  positions_abs

%block species
O    O    8    4    6.5
C    C    6    4    6.5
H    H    1    1    6.5
%endblock species

%block species_pot
O    oxygen.recpot
C    carbon.recpot
H    hydrogen.recpot
%endblock species_pot
```



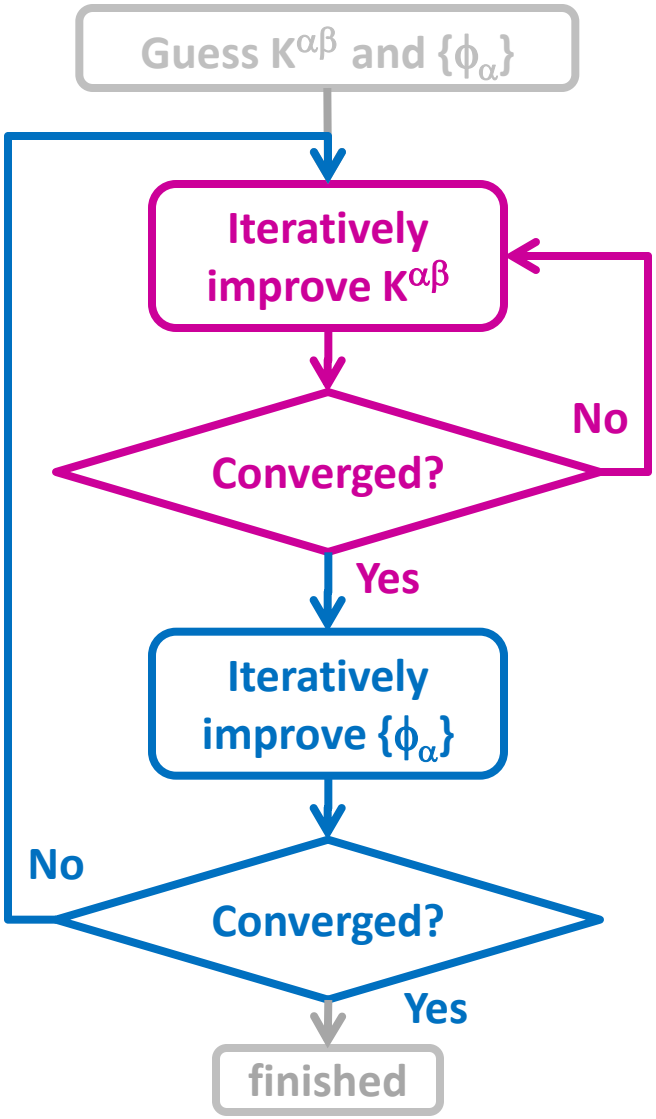
ONETEP calculation outline

- 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) density kernel using canonical purification
  - Refine initial density kernel (self-consistently) using penalty functional



ONETEP calculation 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) using Density Matrix Minimisation approaches



Example output file: formaldehyde

```
+-----------------------------------------------------------------+
|                                                                 |
|        ####### #     # ####### ####### ####### ######          |
|        #     # ##    # #           #    #       #     #         |
|        #     # # #   # #           #    #       #     #         |
|        #     # #  #  # #####       #    #####   ######          |
|        #     # #   # # #           #    #       #               |
|        #     # #    ## #           #    #       #               |
|        ####### #     # #######     #    ####### #               |
|                                                                 |
|        Linear-Scaling Ab Initio Total Energy Program            |
|                                                                 |
|          Release for academic collaborators of ODG              |
|                                            Version 3.5.2.9      |
|                                                                 |
+-----------------------------------------------------------------+
|                                                                 |
|  Authors:                                                       |
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|  Arash. A. Mostofi, Mike C. Payne and Chris-Kriton Skylaris     |
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|  Contributors:                                                  |
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|  O. Dieguez, S. M. M. Dubois, H. H. Helal, Q. O. Hill,          |
|  D. D. O`Regan, C. J. Pickard, L. P. Lee, M. I. J. Probert,     |
|  L. Ratcliff, M. Robinson, A. Ruiz Serrano, J. S. Spencer,      |
|  G. Teobaldi, K. A. Wilkinson and T. J. Zuehlsdorff             |
|                                                                 |
|                                   Copyright (c) 2004-2013       |
```
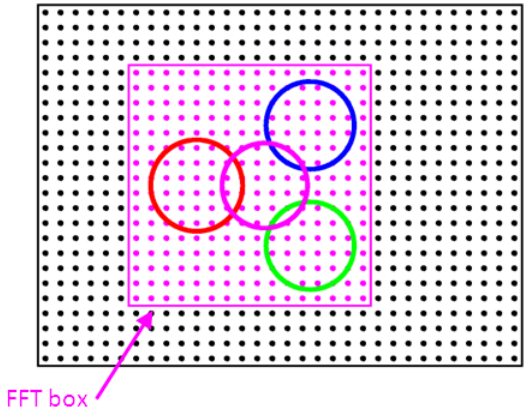

Example output file: formaldehyde

- Parallel strategy, calculation parameters

```
Reading parameters from file "h2co.dat" ...... done
Running on     2 processors.
There are   2 MPI processes running on the same node as the root process.
Each MPI process is using:
             1 threads for simulation cell FFTs.
             1 threads for parallel FFT box operations.
             1 threads for loops over batched FFT box operations.
             1 threads in other parallel regions.

Reading geometry and species blocks from file "h2co.dat" ...
  <species_atomic_set> block not found: NGWF initialisation set to SOLVE
... done
------------------------------------------------------------------------------
---------------------------- RUN-TIME PARAMETERS -----------------------------
------------------------------------------------------------------------------
task                        : SINGLEPOINT *! Type of calculation (String)
cutoffenergy                : 22.0493965347193      hartree *! Plane wave kineti
kernelcutoff                : 1000.00000000000      bohr *! Density kernel radiu
xcfunctional                : LDA *! Exchange-correlation functional (String)
```

Example output file: formaldehyde

```
------------------------- Atom counting information ---------------------------
Symbol     Natoms     Ngwfs     Nprojs
  O          1          4          1
  C          1          4          1
  H          2          2          0
.......    ......     ......     ......
Totals:      4         10          2
-------------------------------------------------------------------------------

============================== PSINC grid sizes ================================
                      Simulation cell:   84 x  84 x  84
                              FFT-box:   75 x  75 x  75
                                  PPD:    6 x   6 x   1
Grid space d1=  0.571428571429a0 (KE cutoff=  23.26377Eh = 633.03940eV)
Grid space d2=  0.571428571429a0 (KE cutoff=  23.26377Eh = 633.03940eV)
Grid space d3=  0.571428571429a0 (KE cutoff=  23.26377Eh = 633.03940eV)
===============================================================================
```



- Simulation cell, FFT box, grid spacing

Example output file: formaldehyde

- NGWF initialisation to pseudo-atomic orbitals (PAOs)

```
Atom SCF Calculation for O  : Z (AE atom) =   8 : Z (PS atom) =   6
Config String:
Orbitals (num,occ):  2     2.00 4.00
Orbitals   (num,l):  2        0    1
Atom SCF converged after  33 iterations to a total energy of    -15.71589674

Atom SCF Calculation for C  : Z (AE atom) =   6 : Z (PS atom) =   4
Config String:
Orbitals (num,occ):  2     2.00 2.00
Orbitals   (num,l):  2        0    1
Atom SCF converged after  33 iterations to a total energy of     -5.33577996

Atom SCF Calculation for H  : Z (AE atom) =   1 : Z (PS atom) =   1
Config String:
Orbitals (num,occ):  1     1.00
Orbitals   (num,l):  1        0
Atom SCF converged after  30 iterations to a total energy of     -0.43623914
NGWF initialisation ...... done
```

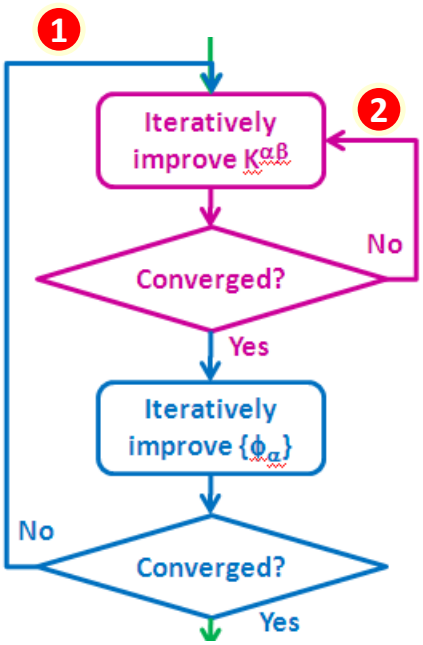
Example output file: formaldehyde

- Initialise and refine density kernel

```
Up spin density kernel initialisation ...... done

Writing density kernel to file "h2co.dkn" ... done
...............................................................................
<<<<<<<<<<<<<<<< Penalty functional density kernel optimisation >>>>>>>>>>>>>>>>
~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
iter|       energy      |   rms grad  |  commutator |LScoef|CGcoef|      Ne    |
 1    -22.30601581980334 0.20331628150 0.04484007235 0.0375  0.000   12.00000000
 2    -22.46076257396956 0.14069499042 0.04175487618 1.5516 -0.674   12.00000000
 3    -22.52670521876486 0.14039924989 0.01362266216 0.0597  2.530   12.00000000

======================== Penalty functional minimisation =======================
   Final total energy     :     -22.686005604142
   Final penalty energy   :       0.124364019320
   RMS occupancy error    :       0.055759
   Occupancy bounds       : [-0.073, 1.095]
===============================================================================

Finished density kernel iterations (   3)

Writing density kernel to file "h2co.dkn" ... done
```

Example output file: formaldehyde

- SCF iterations




```
1  ##############################################################################
   ########################### NGWF CG iteration  003 ############################
   ##############################################################################
   ****** Reciprocal space K.E. preconditioning with k_zero =  3.0000 a0^-1 *******
   ..............................................................................
2  <<<<<<<<<<<<<< LNV (Original version) density kernel optimisation >>>>>>>>>>>>>>
   ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~
   iter|       energy       |  rms DeltaK |  commutator |LScoef|CGcoef|      Ne    |
    1    -22.59764463503945 0.00000000000 0.00742800720 0.3105  0.000   12.00000000
    2    -22.59887443008579 0.00006851746 0.00155916919 0.5507  0.044   12.00000000
    3    -22.59897014644941 0.00000556547 0.00042177118 1.0778  0.073   12.00000000
    4    -22.59898529365745 0.00000082140 0.00012592339 0.5328  0.089   12.00000000
    5    -22.59898597853532 0.00000004553 0.00005574035 0.0000  0.000   12.00000000
   Finished density kernel iterations (   5)

   Writing density kernel to file "h2co.dkn" ... done

   ------------------------------ NGWF line search -------------------------------
   RMS gradient                =       0.00052360108010
   Trial step length           =               0.454088
   Gradient along search dir.  =         -0.01771552767
   Functional at step 0        =     -22.59898597853532
   Functional at step 1        =     -22.60468394577041
   Functional predicted        =     -22.60588073836902
   Selected quadratic step     =               0.778386
   Conjugate gradients coeff.  =               0.227644
   --------------------------- NGWF line search finished ---------------------------

   Writing NGWFs to file "h2co.tightbox_ngwfs"....  done

   ##############################################################################
   ########################### NGWF CG iteration  004 ############################
   ##############################################################################
   ****** Reciprocal space K.E. preconditioning with k_zero =  3.0000 a0^-1 *******
   ..............................................................................
```

Example output file: formaldehyde

- End of SCF calculation

```
.....................................................
          | *** NGWF optimisation converged ***                 |
          | RMS NGWF gradient =    0.00000060044935             |
          | Criteria satisfied:                                 |
          | -> RMS NGWF gradient lower than set threshold.      |
          ======================================================

==============================================================================
          ---------------- ENERGY COMPONENTS (Eh) ----------------
          | Kinetic                    :       14.91654726777243 |
          | Pseudopotential (local)    :      -75.55457414479615 |
          | Pseudopotential (non-local):        3.08869996279848 |
          | Hartree                    :       29.55310839834672 |
          | Exchange-correlation       :       -5.51704179513331 |
          | Ewald                      :       10.90369328705708 |
          | Total                      :      -22.60956702395475 |
          -------------------------------------------------------
          Integrated density           :       11.99999999999890
==============================================================================

                    <<<<< CALCULATION SUMMARY >>>>>
|ITER|    RMS GRADIENT    |     TOTAL ENERGY     |   step    |     Epredicted
   1     0.00339839407455    -22.36004521507221   0.577465    -22.56562648226837
   2     0.00109741818065    -22.56841844240503   0.775342    -22.59768200552023
   3     0.00052360108010    -22.59898597853532   0.778386    -22.60588073836902
   4     0.00030634807668    -22.60616555840943   0.779132    -22.60851978307256
   5     0.00017102918908    -22.60861455112408   0.617621    -22.60917144516267
   6     0.00010980625916    -22.60917266853535   0.829103    -22.60948153377710
   7     0.00006521343432    -22.60948683504158   0.578949    -22.60956387837020
   8     0.00000603632378    -22.60956697055239   0.021300    -22.60956699447697
   9     0.00000390750401    -22.60956702082759   0.000047    -22.60956702085166
  10     0.00000388098078    -22.60956702088541   0.003009    -22.60956702376849
  11     0.00000060044935    -22.60956702395475  <-- CG
```

Summary of Functionality

Total energies

- Various exchange-correlation functionals: LDA (Ceperley-Alder-Perdew-Zunger, Vosko-Wilk-Nusair, PW92), GGA (PW91, PBE, revPBE, RPBE, BLYP, XLYP, WC). Also interface with LIBXC which can provide a large variety of functionals.
- Spin polarisation
- DFT+D (empirical dispersion)
- DFT+U
- Charge-constrained DFT
- Non-local exchange-correlation functionals for dispersion (e.g. Langreth and Lundqvist approach)
- Hartree-Fock exchange and hybrid functionals (coming soon)
- Finite temperature DFT for metallic systems

Summary of Functionality

Boundary conditions

- Periodic boundary conditions
- Open boundary conditions (Cut-off Coulomb, Martyna-Tuckerman or real-space open boundaries)
- Implicit solvent model
- Electrostatic embedding

Core electrons

- Norm conserving pseudopotentials
- Projector Augmented wave (PAW) approach (all electron)

Summary of Functionality

Atomic forces

- Geometry optimisation
- Transition state search
- Ab initio molecular dynamics

Visualisation

- NGWFs
- Molecular Orbitals
- Density and potentials

Atomic orbitals

- Instead of NGWFs construct and use SZ, SZP, DZ, DZP, etc atomic orbital basis sets

Summary of Functionality

Electronic properties

- Density of states, local density of states
- Atomic charges
- Dipole moments
- Optimisation of separate NGWF set for accurate conduction bands and optical absorption spectra
- Natural Bond Orbital (NBO) analysis (Natural Atomic Orbitals in ONETEP and interface to NBO5.9 program)
- Electron transport

More information

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

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