Workshop on
Application of Density-Functional Theory in
Condensed-Matter Physics, Surface Physics, Chemistry,
Engeneerging, and Biology

Berlin, 21- 30 July 2003

Introduction to SFHIngX[1]

Simulation package of the
Fritz-Haber-Institute / junior group
called SFHIngX

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[1] http://www.sfhingx.de

Introduction to SFHIngX

DFT codes: basis-sets/methods (PW, Gaussian, LCAO, wavelets, ...)
(FP-LAPW, PP, PAW, ...)

New Methods:
- improvement of conventional DFT calculations
  e.g. band gap problem, excited states, ...
- larger system sizes, better scaling behavior, multi-scale

Problem: codes 10.000 – 500.000 lines of code
hard to maintain
developing/testing of new approaches rather complex

Solution: modular DFT library rather than DFT code

Goal: DFT developer's framework
User friendly

Modular DFT library rather than DFT code

FORTRAN77:

+ very fast code
- not modular, hard to maintain
- static memory management
- no user types

FORTRAN 90/95:

+ fast
  (scalar access)
± modular, no object-orientation
+ dynamic memory management
- compiler not reliable yet
  (e.g. IBM: xlF – numerically instable,
  HP: f90 – difficulties with pointers)

C/C++:

- 1.3 ... 3 times slower than F77
  (due to scalar operations)
+ object orientated → smaller source code
+ type safe
+ standardized language and compilers
  (ANSI, POSIX)

The best of both worlds - Speeding up C/C++

$$\alpha\mathbf{A} + \beta\mathbf{B} + \gamma\mathbf{C}^{-1}$$

"cheating!!!"
Multi language mixing

```
Matrix M, A=..., B=..., C=...;
M = a*A + b*B + g*C.inverse();
```

C/C++ overloading of operators

C/C++

BLAS/LAPACK function call replacement
at compile time

```
call DAXPY (a, A)
...
call htridi(C)
...
call DAXPY (a, M)
```

C or FORTRAN
numerical libraries
(BLAS/LAPACK)

Class Hierarchy

DFT tier

Hamiltonian Solver
(SD, WS, DJ, CCG, DIIS_CCG)

Hamiltonian
(H, ξ=-HΨ,E, F, ε, ...,)

PW-Basis

Bloch Wavefunctions

cross platform tier

Template library class
(+,-,*,/,Ma=mx,M^{-1},...)

File I/O
(ASCII, binary)

TCP/IP
communication

platform dependent tier

numeric interface
(+,-,*,/,Ma=mx,M^{-1},...)

FORTRAN or C BLAS/LAPACK library
ATLAS, IBM-ESSL, HP-VecLIB, ...

Tool
netCDF library, strings, exceptions

Sockets
network, server, clients

Class Hierarchy

SFHIngX
ab-initio DFT code

SFHIngX add-ons
many small helper tools
controlling, analysis, visualization...

structure tier

Struct. optim.
damped Newton,
quasi Newton

Trans. state search

Frozen Phonons

***ab-initio* MD**

DFT tier

Hamiltonian Solver
(SD, WS, DJ, CCG, DIIS_CCG)

Hamiltonian
(H, ξ=-HΨ,E, F, ε, ...,)

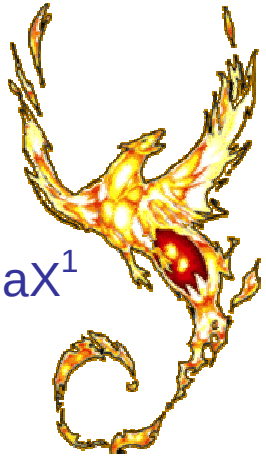
PW-Basis

Bloch Wavefunctions

SFHIngX – user interface

Input file: hierarchical and modular structure
scriptable
customizable grammar and range checker
customizable structure and PP database

Interactions: TCP/IP network communications via
- telnet session
- web/wap interface IsiX
- graphical user interface PHInaX[1]



Analysis: Many small add-ons
incl. 3d visualization
- atomic structures
- isodensities, contour slices

[1] http://www.phinax.de

SFHIngX – input file

```
format sfhingx;
aLat = 10.68;  # Bohr
structure  {
   include <structures/fcc.sx>;
   species  {
      potential     = “ga.cpi”;
      name          = “Gallium”;
      valenceCharge = 3;
      ...
   }
   species  {
      potential     = “as.cpi”;
      name          = “Arsenic”;
      valenceCharge = 5;
      ...
   }
   ...
}
```

~/SFHIngX/structures/fcc.sx

SFHIngX – input file

```
format sfhingx;
aLat = 10.68;  # Bohr
structure  {
   include <structures/fcc.sx>;
   species  {
      potential     = “ga.cpi”;
      name          = “Gallium”;
      valenceCharge = 3;
      ...
   }
   species  {
      potential     = “as.cpi”;
      name          = “Arsenic”;
      valenceCharge = 5;
      ...
   }
   ...
}
```

~/SFHIngX/species/ga.sx

SFHIngX – input file

```
format sfhingx;
aLat = 10.68;  # Bohr
structure  {
   include <structures/fcc.sx>;

   include <species/ga.sx>;

                                          ~/SFHIngX/species/zincblende.sx

   include <species/as.sx>;

   ...
}
```

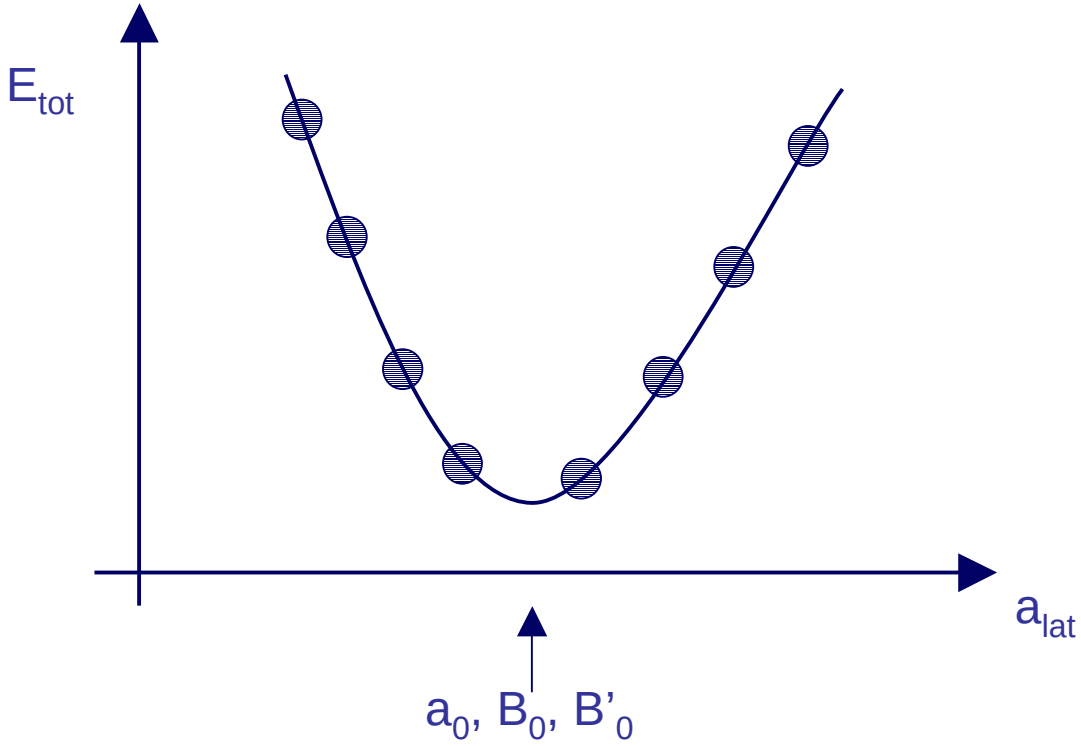
SFHIngX – input file database

$HOME/	SFHIngX/	species/	ga.sx as.sx ...	include <species/ga.sx>;
		potentials/	ga.cpi as.cpi ...	potential = <potentials/ga.cpi>;
		bravais/	fcc.sx bcc.sx ...	include <bravais/fcc.sx>;
		structures/	zincblende.sx diamond.sx ...	include <structures/diamond.sx>;

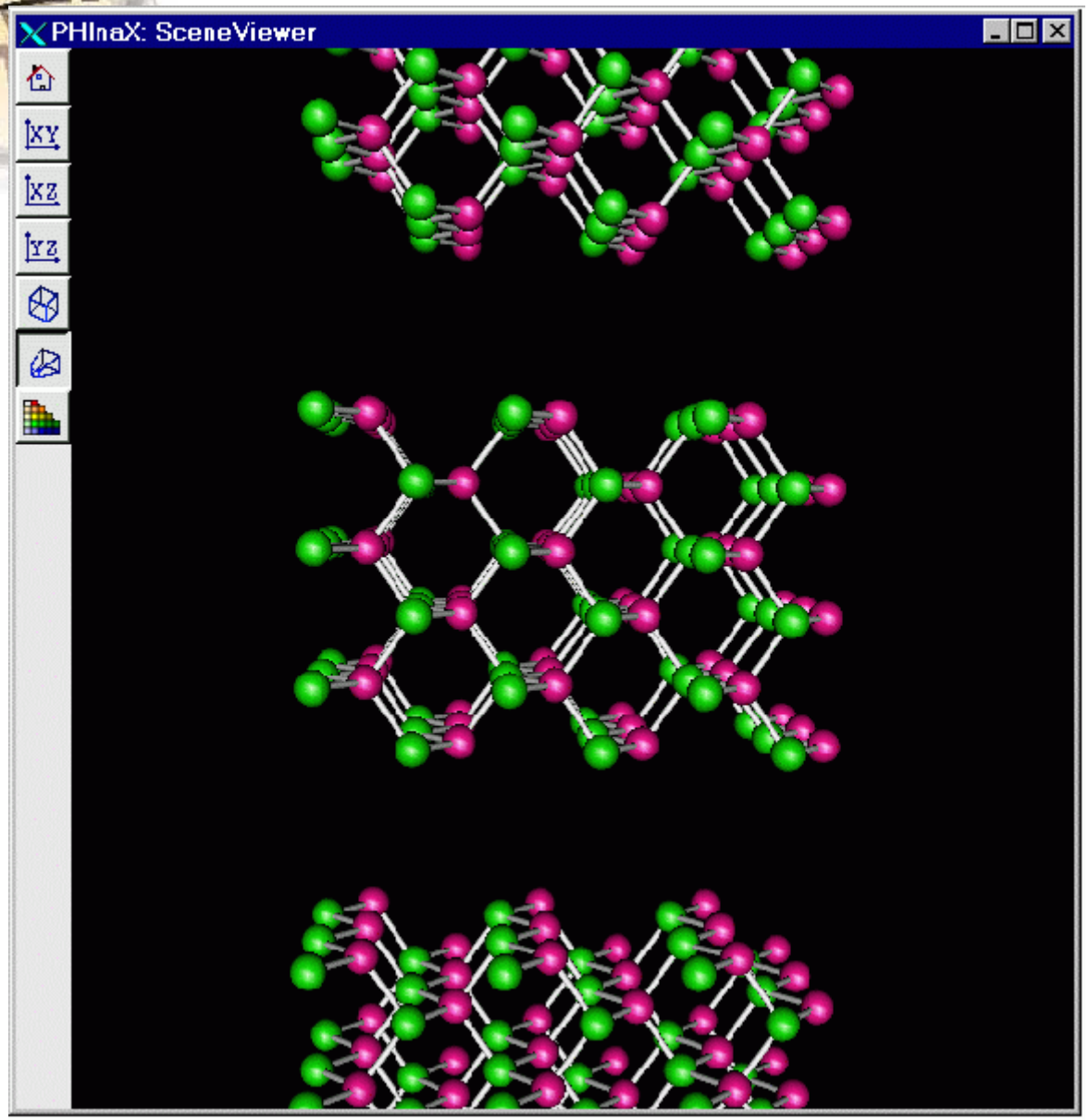
SFHIngX – add ons

Murnaghan fit:

sxmurn



SFHIngX – add ons

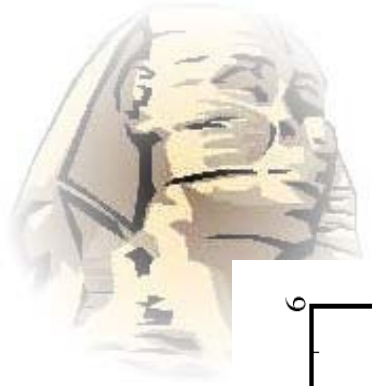


3d visualization

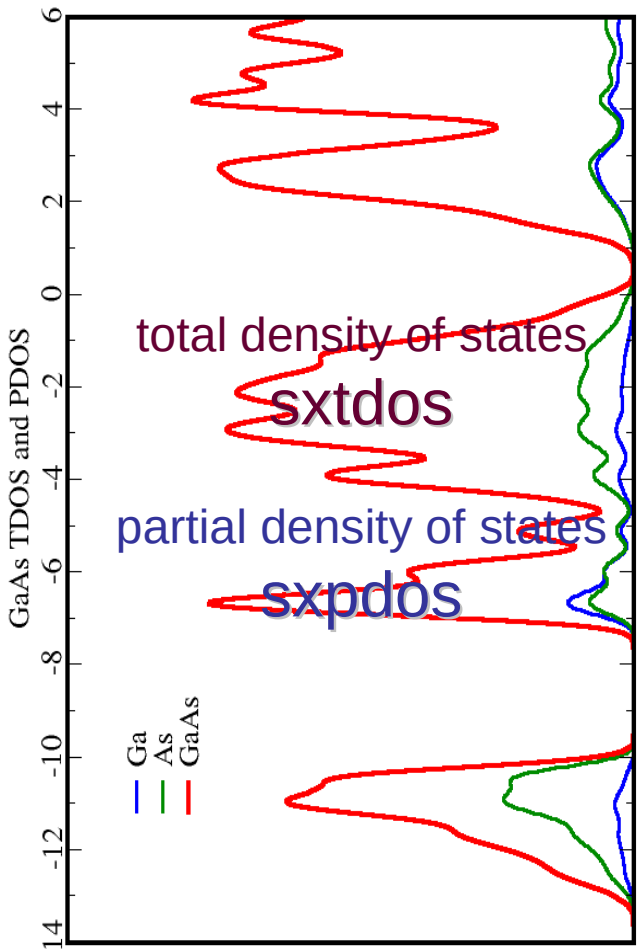
pxviewer

PDB file converter
repating supercell

sx2pdb –r 1x1x3



SFHIngX – add ons

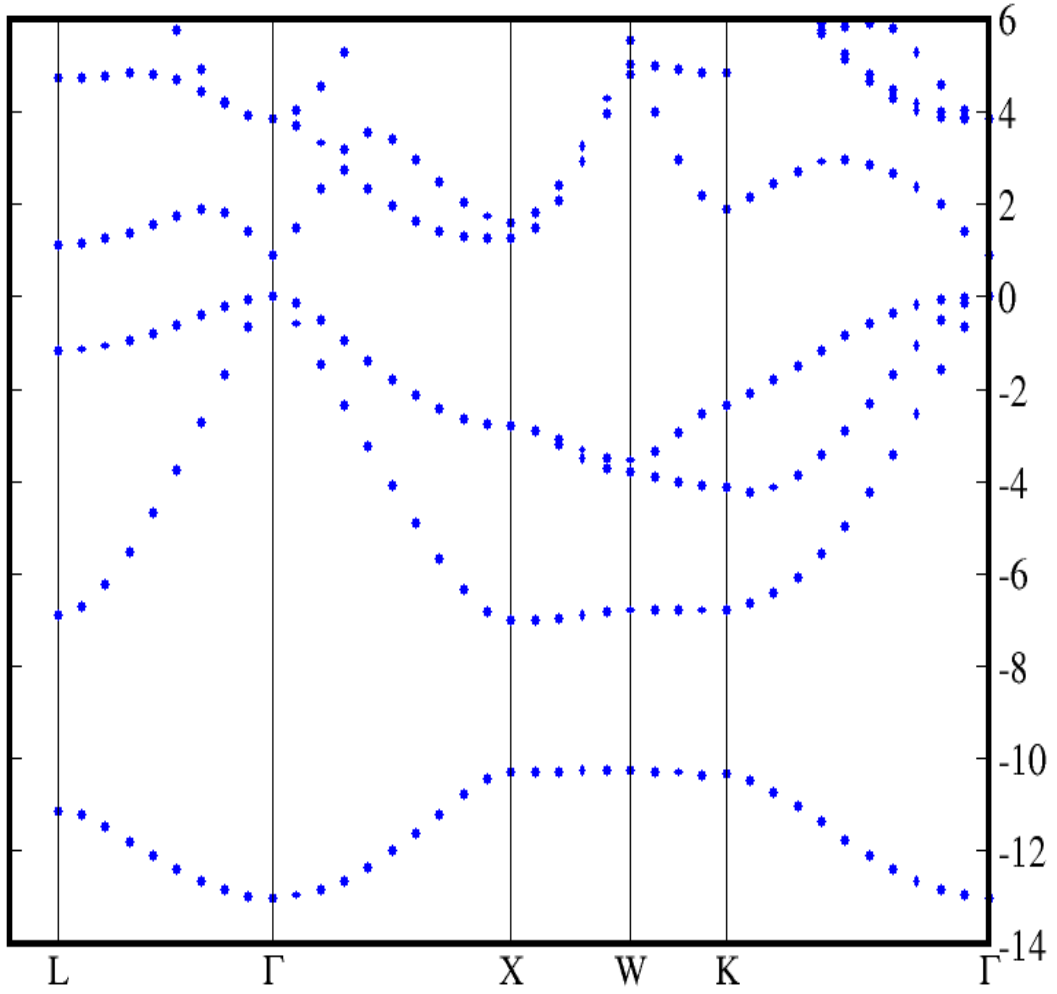


total density of states

sxtdos

partial density of states

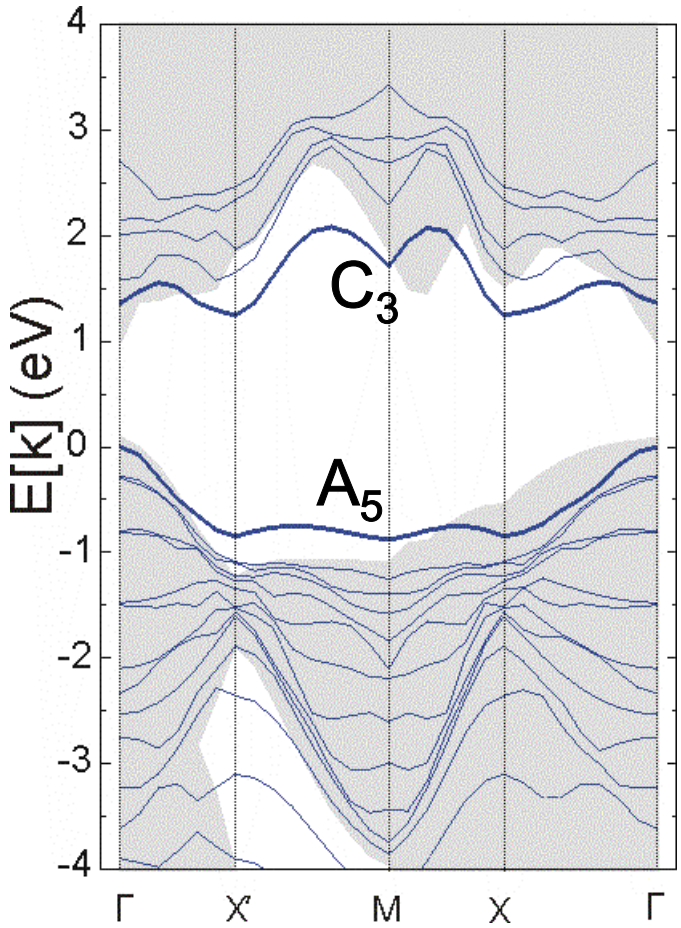
sxpdos

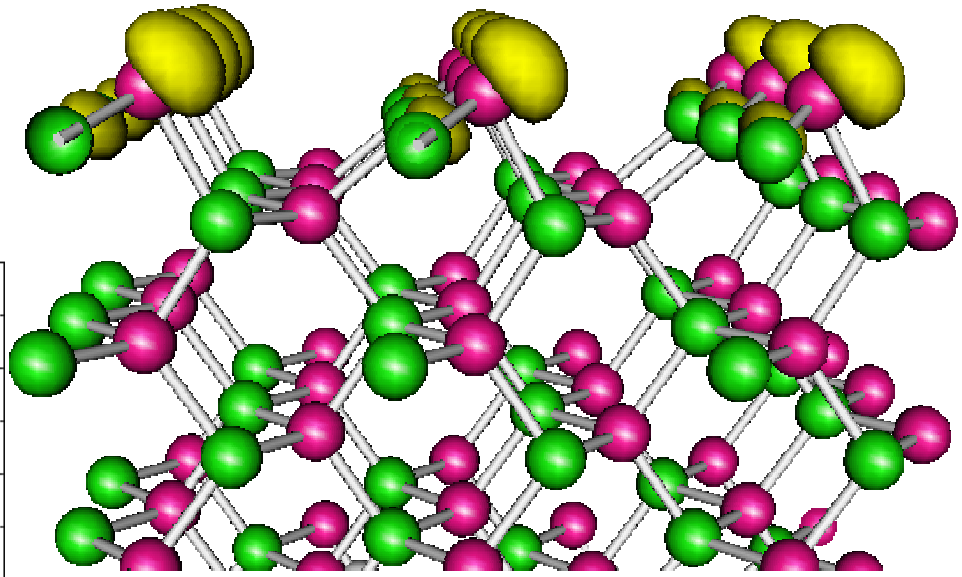


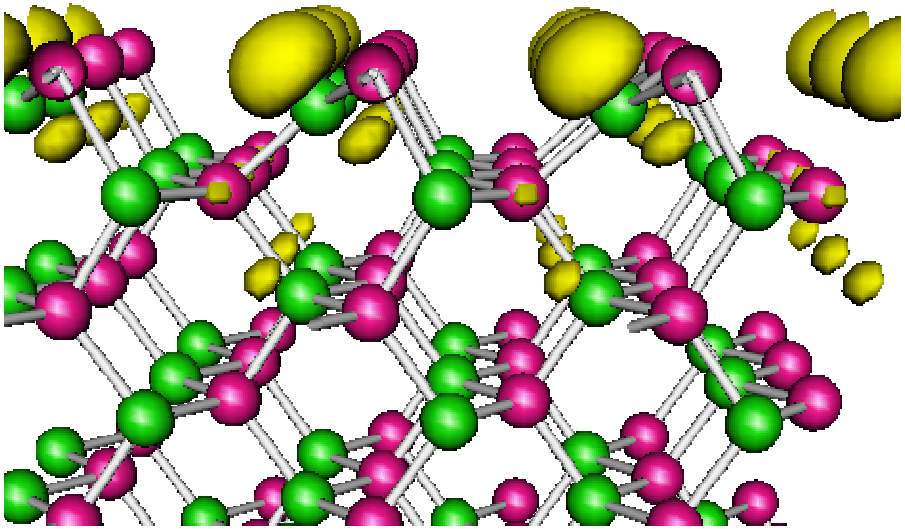
SFHIngX – add ons

partial charge density

sxpartialrho





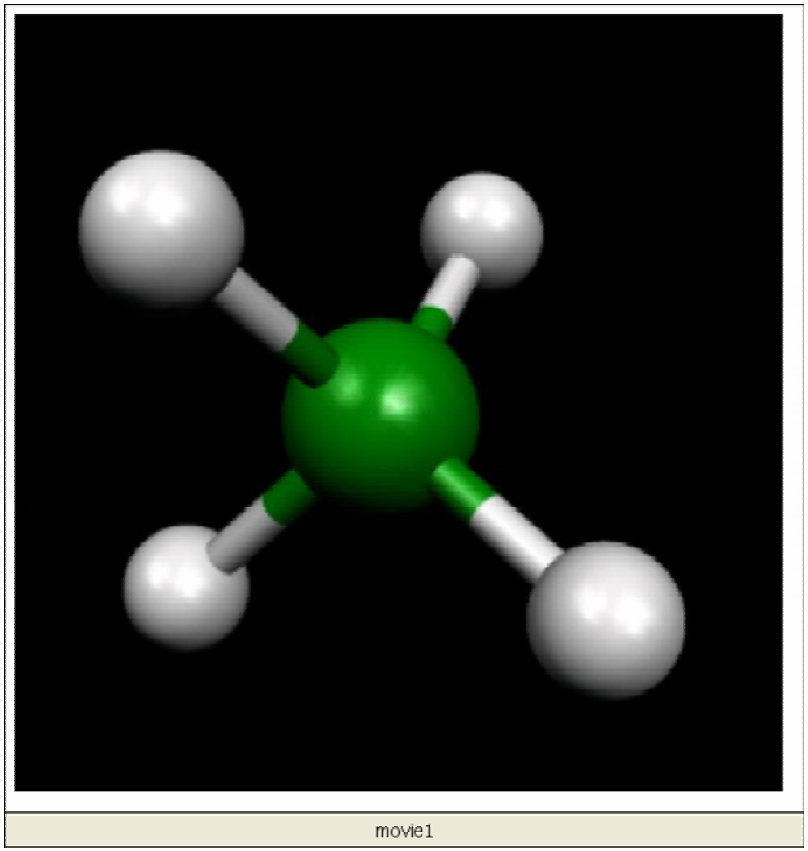


SFHIngX – add ons

MD run

MD trajectory to MOLDEN converter
sxhist2molf

visualization



SFHIngX – add ons

sxatmom	atomic moment
sxconv	struct. format converter
sxdifrho	rho differences
sxget	get simple data
sxgetdyn	thermodyn. analysis
sxhist2corr	calc. correlation from MD
sxhist2molf	Molden converter
sxlogplot	log. plot. converter
sxmeshline	mesh average along line
sxmulliken	Mulliken population
sxmurn	Murnaghan fit
sxpartialrho	partial charge density
sxpdos	proj. DOS
sxprint	print input file
sxrepeatrho	repeat 3d meshes
sxrhodiv	mesh / constant
sxrhominus	mesh - constant
sxrhomult	mesh * constant
sxrhoplus	mesh + constant
sxrhospin	get spin density
sxrhosplit	split spin channels
sxsumrho	sum meshes
sxtdos	total DOS
sxwavetransfer	waves.sxb converter

... and many other more ...

Summary

SFHIngX = modular **DFT library** and a **DFT code**
fewer code lines

supported platforms:

- Linux
- HP (n class machines)
- IBM (Regatta SP4)
- Win32

User interface:

- Hierarchical input file with algebra evaluation capabilities
- many small add-ons
- TCP/IP communication (web interface: IsiX)
- Graphical User Interface (PHInaX)

Current Implementation:

Plane-waves, pseudopotential code
electronic minimization schemes: DJ, all-state + state CG
structure optimization: damped + quasi Newton
ab-initio MD
transition state search

Class Hierarchy

DFT tier

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(SD, WS, DJ, CCG, DIIS_CCG)

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PW-Basis

Bloch Wavefunctions

cross platform tier

Template library class
(+,-,*,/,Ma=mx,M^{-1},...)

File I/O
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platform dependent tier

numeric interface
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FORTRAN or C BLAS/LAPACK library
ATLAS, IBM-ESSL, HP-VecLIB, ...

Tool
netCDF library, strings, exceptions

Sockets
network, server, clients

Class Hierarchy

DFT tier

Hamiltonian Solver
(SD, WS, DJ, CCG, DIIS_CCG)

Hamiltonian
(H, ξ=-HΨ,E, F, ε, ...,)

Dirac tier

Dirac Basis
R, r, G, G+k, ...
Metric, Scalar product

Dirac Wavefunctions
Ψ, μ, ...
Vector representation

cross platform tier

Template library class
(+,-,*,/,Ma=mx,M^{-1},...)

File I/O
(ASCII, binary)

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FORTRAN or C
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Tool
netCDF library,
strings, exceptions

Sockets
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Code snippets

```
SxRBasis   R (mesh, geom);
SxGBasis   G (mesh, geom, eCut);
SxGkBasis  Gk (G, kp, weights, folding, eCut);
SxRadBasis r;

SxPWSet waves(nStates, nSpin, Gk);

SxRBasis::TPsi psiG = waves(0, 0, 0);
```

$|\mathbf{R}\rangle$ $|\mathbf{G}\rangle$ $|\mathbf{G}+\mathbf{k}\rangle$ $|r\rangle$ $|\Psi\rangle$ $\langle \mathbf{G}+\mathbf{k}|\Psi_{i\sigma\mathbf{k}}\rangle$

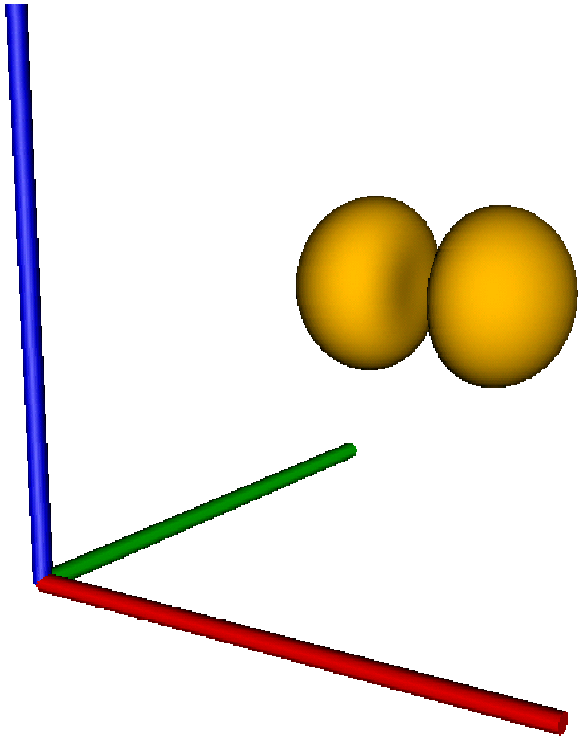
Σ_{G+k_0} $\langle R \mid G+k_0 \rangle$ $\langle G+k_0 \mid \Psi \rangle$

```
psiR = SUM (Gk(0), (R | Gk(0)) * (Gk(0) | psiG);
```

$\langle R \mid \Psi \rangle$

```
psiR = (R | psiG);
```

Code snippets



```
SxRBasis   R  (mesh, str);
SxGBasis   G  (mesh, str, gCut);
SxGkBasis  Gk (G, kp, weights, eCut);
SxRadBasis r  (pseudoRad, omega);

SxOrbitals orbs (pseudoPsi, r);

R.writeMesh3d("dz2.sxb",
   SUM(G,((R|G)*(G|orbs(is,ia,n,s, 0))).absSqr()
);
```

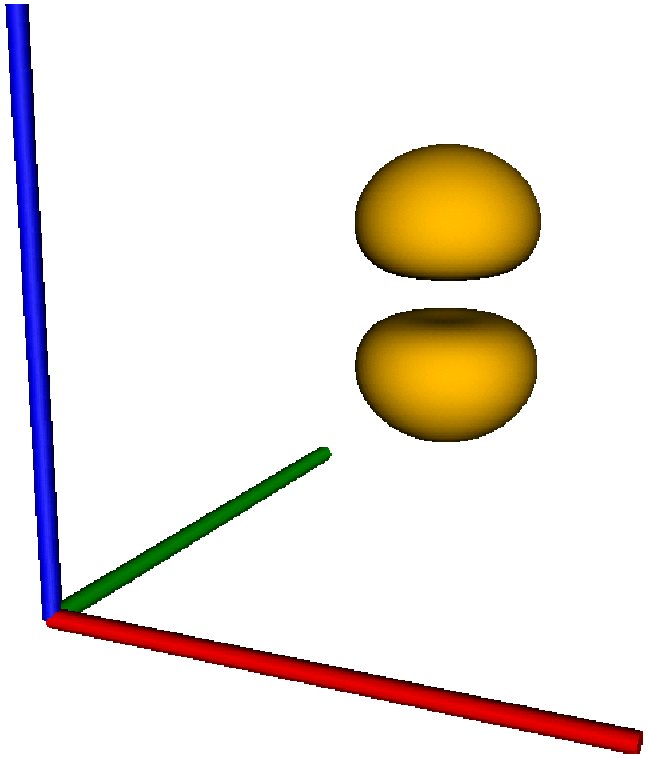
$|\mathbf{R}\rangle$
$|\mathbf{G}\rangle$
$|\mathbf{G}+\mathbf{k}\rangle$
$|r\rangle$

$\langle r|\mu\rangle$

$$\left\| \sum_{\mathbf{G}} \langle \mathbf{R}|\mathbf{G}\rangle \langle \mathbf{G}|\mu_{is,ia,n,l,m}\rangle \right\|^2$$

p_x

Code snippets



```
SxRBasis   R  (mesh, str);
SxGBasis   G  (mesh, str, gCut);
SxGkBasis  Gk (G, kp, weights, eCut);
SxRadBasis r  (pseudoRad, omega);

SxOrbitals orbs (pseudoPsi, r);

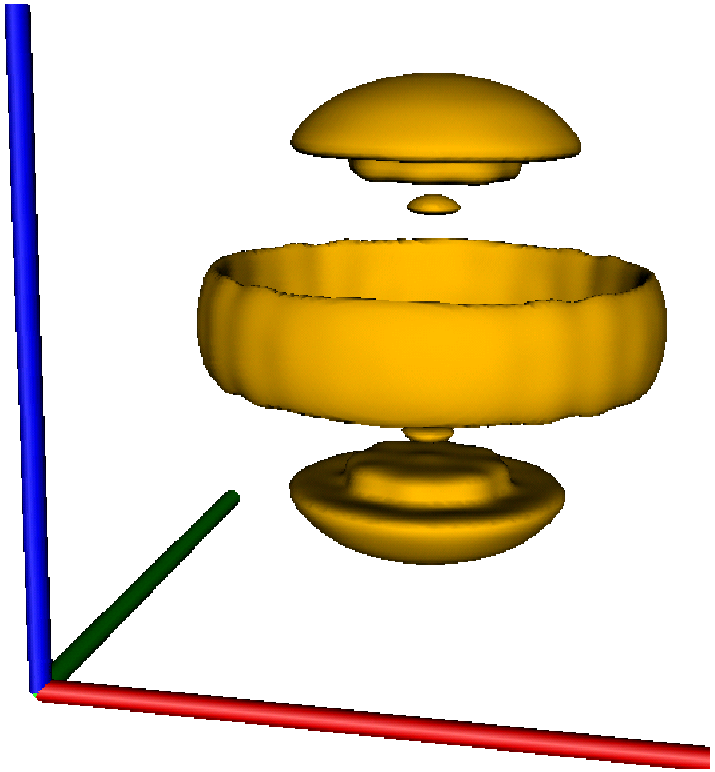
R.writeMesh3d("dz2.sxb",
   SUM(G,((R|G)*(G|orbs(is,ia,n,p,-1)))).absSqr()
);
```

$|\mathbf{R}\rangle$
$|\mathbf{G}\rangle$
$|\mathbf{G}+\mathbf{k}\rangle$
$|r\rangle$

$\langle r|\mu\rangle$

p_z

Code snippets



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SxRBasis   R  (mesh, str);
SxGBasis   G  (mesh, str, gCut);
SxGkBasis  Gk (G, kp, weights, eCut);
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SxOrbitals orbs (pseudoPsi, r);

R.writeMesh3d("dz2.sxb",
   SUM(G,((R|G)*(G|orbs(is,ia,n,d, 2)))).absSqr()
);
```

$|\mathbf{R}\rangle$
$|\mathbf{G}\rangle$
$|\mathbf{G}+\mathbf{k}\rangle$
$|r\rangle$

$\langle r|\mu\rangle$

d_z^2

Credits

Supervision	Jörg Neugebauer
SFHIngX Algebra Libraries DFT Basis Electronic Minimization	Sixten Boeck
Exact Exchange Formalism	Abdullah Alsharif, Abdallah Qteish
Structure Optimization Transition State Search Frozen Phonons Molecular Dynamics	Lars Ismer
Spin polarization Handling metallic systems Real space Projectors electronic analysis	Alexey Dick
chemical analysis tools GWST Interface	Christoph Freysoldt