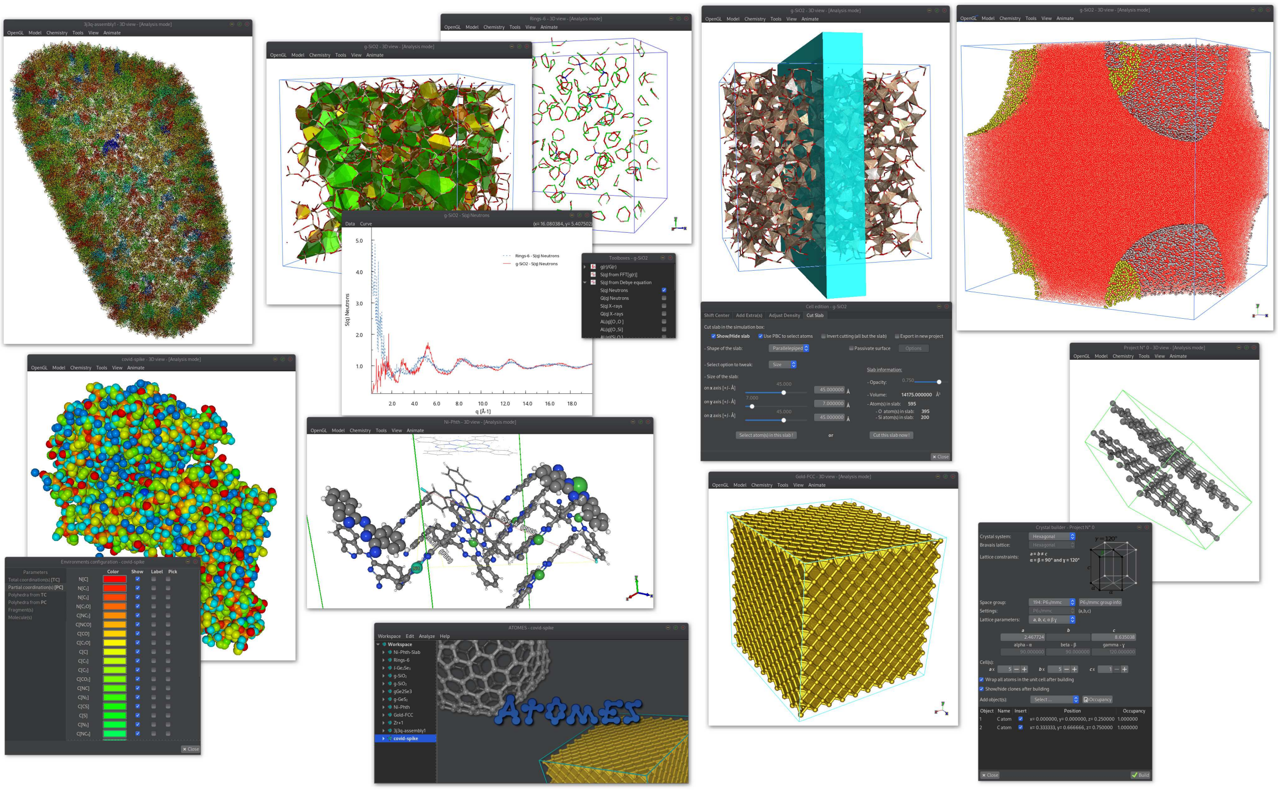
atomes

https://atomes.ipcms.fr



atomes tutorials

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Introduction

This documents regroups tutorials to help user discover the capabilities of the **atomes** program.
Tutorials cover many aspects of **atomes** capabilities:

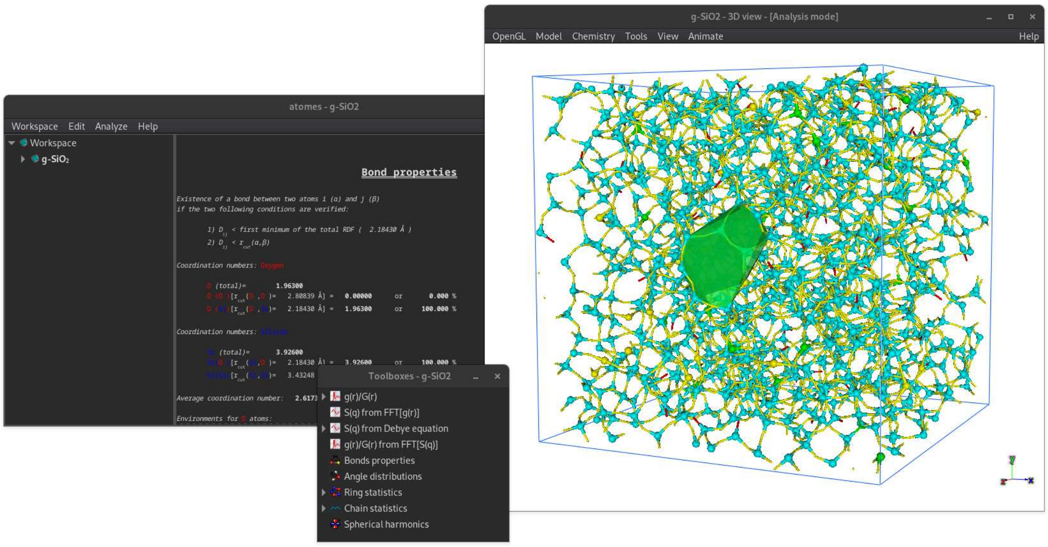
- Getting information on selected structural features: g(r) in *g*-SiO_2.
- Building a crystal, then creating and passivating a surface.

Getting information on selected structural features: g(r) in *g*-SiO$_2$

The following example illustrates how **atomes** can be use to retrieve information on selected structural features:

2.1 Open the atomes g-SiO$_2$ project file

Open the **atomes** project file for the system "*g*SiO$_2$ with ring statistics and custom color map, 3000 atoms"

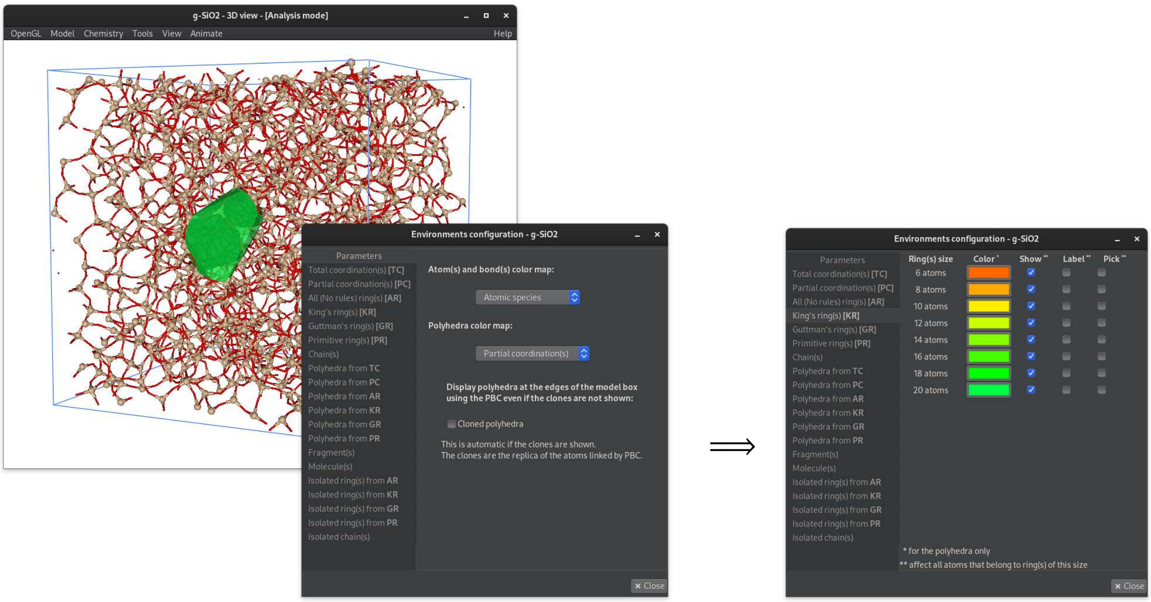

g-SiO2 - 3D view - [Analysis mode]
OpenGL
Model
Chemistry
Tools
View
Animate
Help
atomes - g-SiO2
Workspace
Edit
Analyze
Help
Workspace
g-SiO₂
Toolboxes - g-SiO2
g(r)/G(r)
S(q) from FFT[g(r)]
S(q) from Debye equation
g(r)/G(r) from FFT[S(q)]
Bonds properties
Angle distributions
Ring statistics
Chain statistics
Spherical harmonics

```
Bond properties

Existence of a bond between two atoms i (α) and j (β)
if the two following conditions are verified:

      1) D_ij < first minimum of the total RDF (  2.18430 Å )
      2) D_ij < r_cut(α,β)

Coordination numbers: Oxygen

      O (total)=       1.96300
      O (O )[r_cut(O ,O )=   2.80839 Å] =   0.00000     or      0.000 %
      O (Si)[r_cut(O ,Si)=   2.18430 Å] =   1.96300     or    100.000 %

Coordination numbers: Silicon

      Si (total)=      3.92600
      Si(O )[r_cut(Si,O )=   2.18430 Å] =   3.92600     or    100.000 %
      Si(Si)[r_cut(Si,Si)=   3.43248

Average coordination number:   2.617

Environments for O atoms:
```

Note that the "`Toolboxes`" dialog is active and some results, from calculation performed previously and stored in the project file, are available, including for the radial distribution function g(r).

2.2 Open the "`Environment configuration`" window

Go back to the 3D window of the *g*-SiO_2 model, for clarity purpose change color map to standard chemical species: from the "`OpenGL -> Color Scheme(s)`" menu, or press a as many times as required. Then open the "`Environments configuration`" window: from the "Chemistry" menu or press Ctrl + e , and open the tab labelled "`King’s ring(s)`**[KR]**".


g-SiO2 - 3D view - [Analysis mode]
OpenGL
Model
Chemistry
Tools
View
Animate
Help
Environments configuration - g-SiO2
Parameters
Total coordination(s) [TC]
Partial coordination(s) [PC]
All (No rules) ring(s) [AR]
King's ring(s) [KR]
Guttman's ring(s) [GR]
Primitive ring(s) [PR]
Chain(s)
Polyhedra from TC
Polyhedra from PC
Polyhedra from AR
Polyhedra from KR
Polyhedra from GR
Polyhedra from PR
Fragment(s)
Molecule(s)
Isolated ring(s) from AR
Isolated ring(s) from KR
Isolated ring(s) from GR
Isolated ring(s) from PR
Isolated chain(s)
Close
⟹

Atom(s) and bond(s) color map: Atomic species

Polyhedra color map: Partial coordination(s)

Display polyhedra at the edges of the model box using the PBC even if the clones are not shown:

☐ Cloned polyhedra

This is automatic if the clones are shown.
The clones are the replica of the atoms linked by PBC.

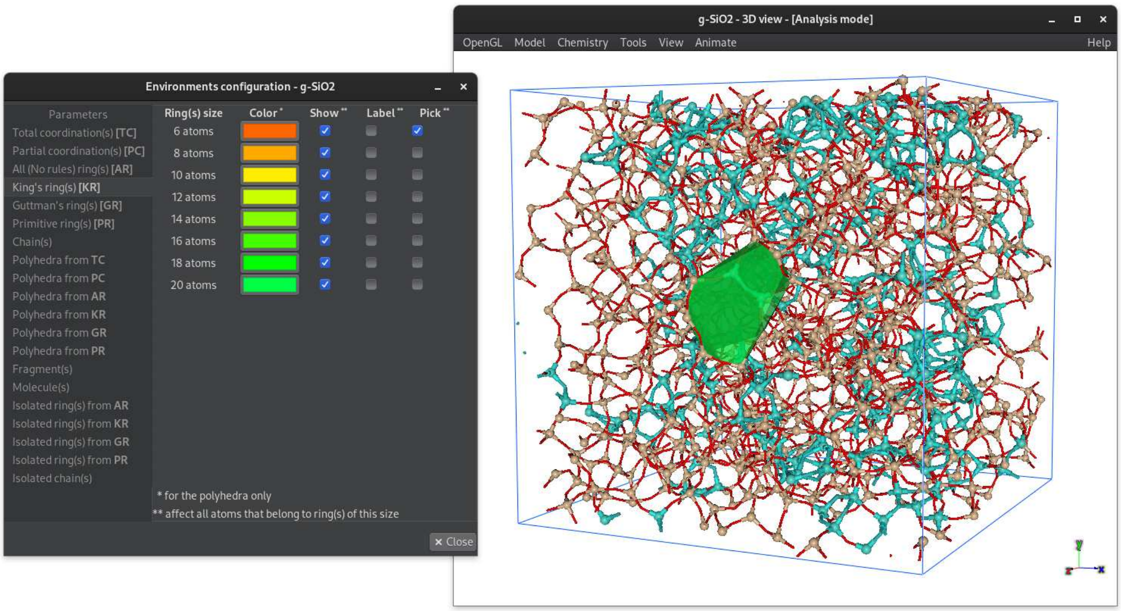
Ring(s) size	Color *	Show **	Label **	Pick **
6 atoms	🟧	☑	☐	☐
8 atoms	🟧	☑	☐	☐
10 atoms	🟨	☑	☐	☐
12 atoms	🟨	☑	☐	☐
14 atoms	🟩	☑	☐	☐
16 atoms	🟩	☑	☐	☐
18 atoms	🟩	☑	☐	☐
20 atoms	🟩	☑	☐	☐

* for the polyhedra only
** affect all atoms that belong to ring(s) of this size

This tab provides interactors with King’s ring statistics calculation results: color of the ring’s polyhedra, and then options to show/hide, label/unlabel, or select/unselect atom(s) involved in any ring(s) of the corresponding size.

2.3 Select all atoms in ring(s) of size 6

"`Pick`" all atoms in ring(s) of size 6: atoms in the 3D window are then selected and highlighted in light blue color.

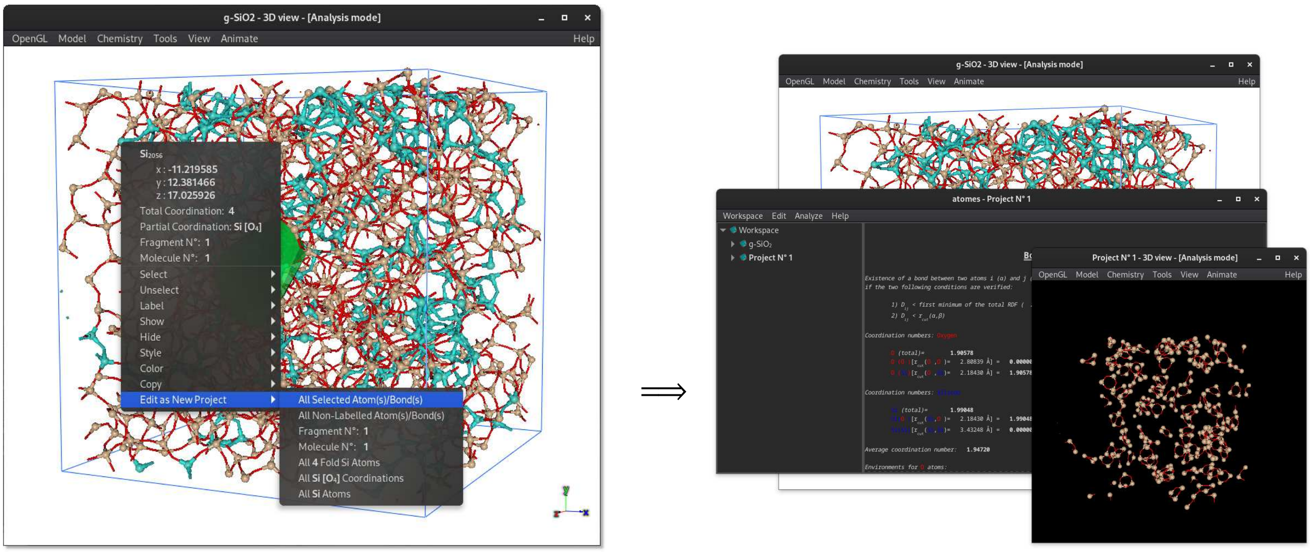

g-SiO2 - 3D view - [Analysis mode]
OpenGL
Model
Chemistry
Tools
View
Animate
Help
Environments configuration - g-SiO2
Parameters
Total coordination(s) [TC]
Partial coordination(s) [PC]
All (No rules) ring(s) [AR]
King's ring(s) [KR]
Guttman's ring(s) [GR]
Primitive ring(s) [PR]
Chain(s)
Polyhedra from TC
Polyhedra from PC
Polyhedra from AR
Polyhedra from KR
Polyhedra from GR
Polyhedra from PR
Fragment(s)
Molecule(s)
Isolated ring(s) from AR
Isolated ring(s) from KR
Isolated ring(s) from GR
Isolated ring(s) from PR
Isolated chain(s)
✕ Close

Ring(s) size	Color *	Show **	Label **	Pick **
6 atoms	🟧	☑	☐	☑
8 atoms	🟧	☑	☐	☐
10 atoms	🟨	☑	☐	☐
12 atoms	🟨	☑	☐	☐
14 atoms	🟩	☑	☐	☐
16 atoms	🟩	☑	☐	☐
18 atoms	🟩	☑	☐	☐
20 atoms	🟩	☑	☐	☐

* for the polyhedra only
** affect all atoms that belong to ring(s) of this size

2.4 Create a new model using the atom selection

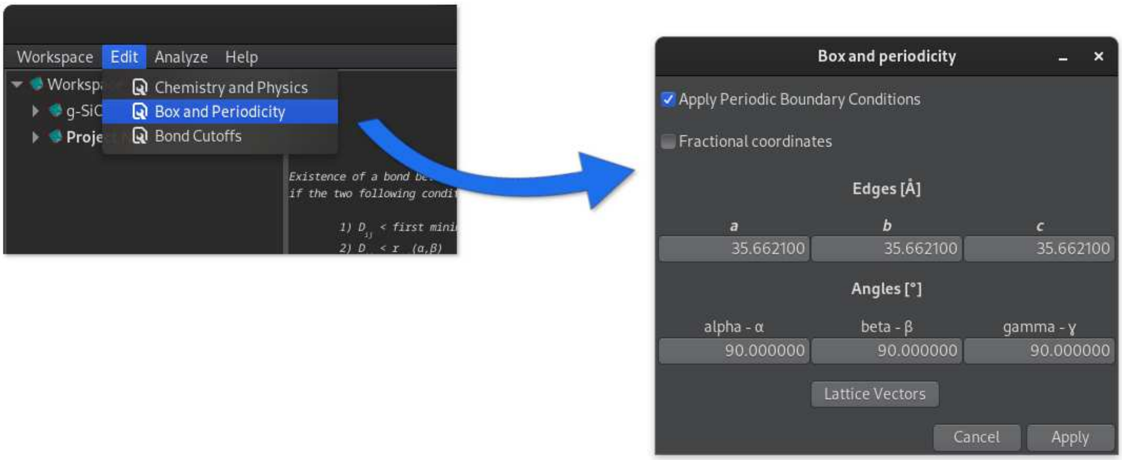
Go back to the 3D window, and mouse right click on any selected atom, then browse the contextual menu that pops up to "`Edit as New Project`", then select "`All Selected Atom(s)/Bond(s)`"


g-SiO2 - 3D view - [Analysis mode]
OpenGL Model Chemistry Tools View Animate Help
Si2056
x : -11.219585
y : 12.381466
z : 17.025926
Total Coordination: 4
Partial Coordination: Si [O$_4$]
Fragment N°: 1
Molecule N°: 1
Select
Unselect
Label
Show
Hide
Style
Color
Copy
Edit as New Project
All Selected Atom(s)/Bond(s)
All Non-Labelled Atom(s)/Bond(s)
Fragment N°: 1
Molecule N°: 1
All 4 Fold Si Atoms
All Si [O$_4$] Coordinations
All Si Atoms
⟹
atomes - Project N° 1
Workspace Edit Analyze Help
Workspace
g-SiO$_2$
Project N° 1
Project N° 1 - 3D view - [Analysis mode]

This will create a new **atomes** project that will immediately be inserted in the program's workspace, and the corresponding 3D window will appear.
This new model contains all atoms involved in King's rings of size 6 selected previously in the disordered SiO_2 model.

2.5 Correct the periodicity of the new model

From the main interface open the "`Edit`" menu and select "`Box and Periodicity`" to reproduce the periodicity of the initial model describing properly the simulation box (a = b = c = 35.6621 Å, $\alpha = \beta = \gamma = 90$ °, and be sure to use Periodic Boundary Conditions), then apply changes.


Workspace
Edit
Analyze
Help
Worksp
g-SiC
Proje
Chemistry and Physics
Box and Periodicity
Bond Cutoffs
Existence of a bond be
if the two following condi
1) D_{ij} < first mini
2) D_{ij} < r (α,β)
Box and periodicity
Lattice Vectors
Cancel
Apply

☑ Apply Periodic Boundary Conditions

☐ Fractional coordinates

Edges [Å]

a	b	c
35.662100	35.662100	35.662100

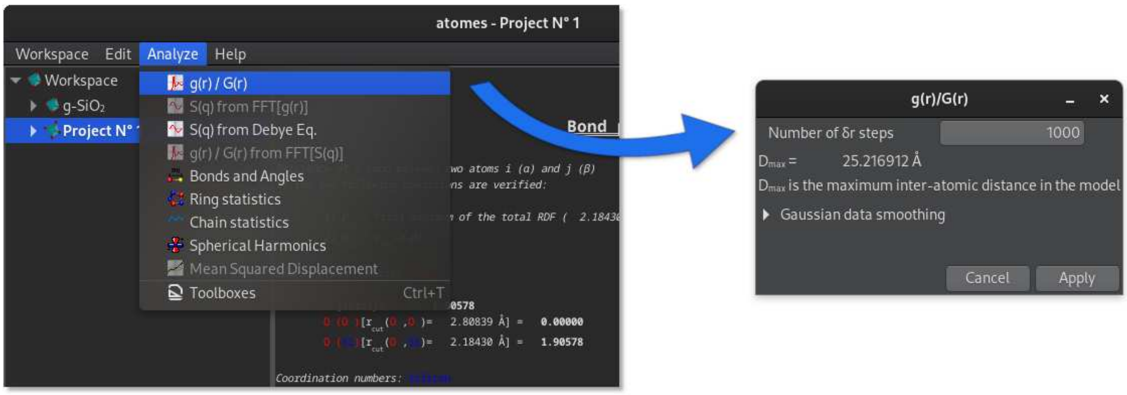
Angles [°]

alpha - α	beta - β	gamma - γ
90.000000	90.000000	90.000000

The new model now uses periodic boundary conditions, if required the box can be displayed in the 3D window using the corresponding menu button: "`Model -> Box -> Show/Hide`".

2.6 Compute the g(r) for the new model

Again from the main interface open the "`Analyze`" menu, then select "`g(r) / G(r)`", to open the associated calculation dialog. Set parameter(s) to acceptable value(s) and run the analysis.


atomes - Project N° 1
Workspace
Edit
Analyze
Help
Workspace
g-SiO₂
Project N° 1
g(r) / G(r)
S(q) from FFT[g(r)]
S(q) from Debye Eq.
g(r) / G(r) from FFT[S(q)]
Bonds and Angles
Ring statistics
Chain statistics
Spherical Harmonics
Mean Squared Displacement
Toolboxes Ctrl+T
Bond
g(r)/G(r)
Gaussian data smoothing
Cancel
Apply

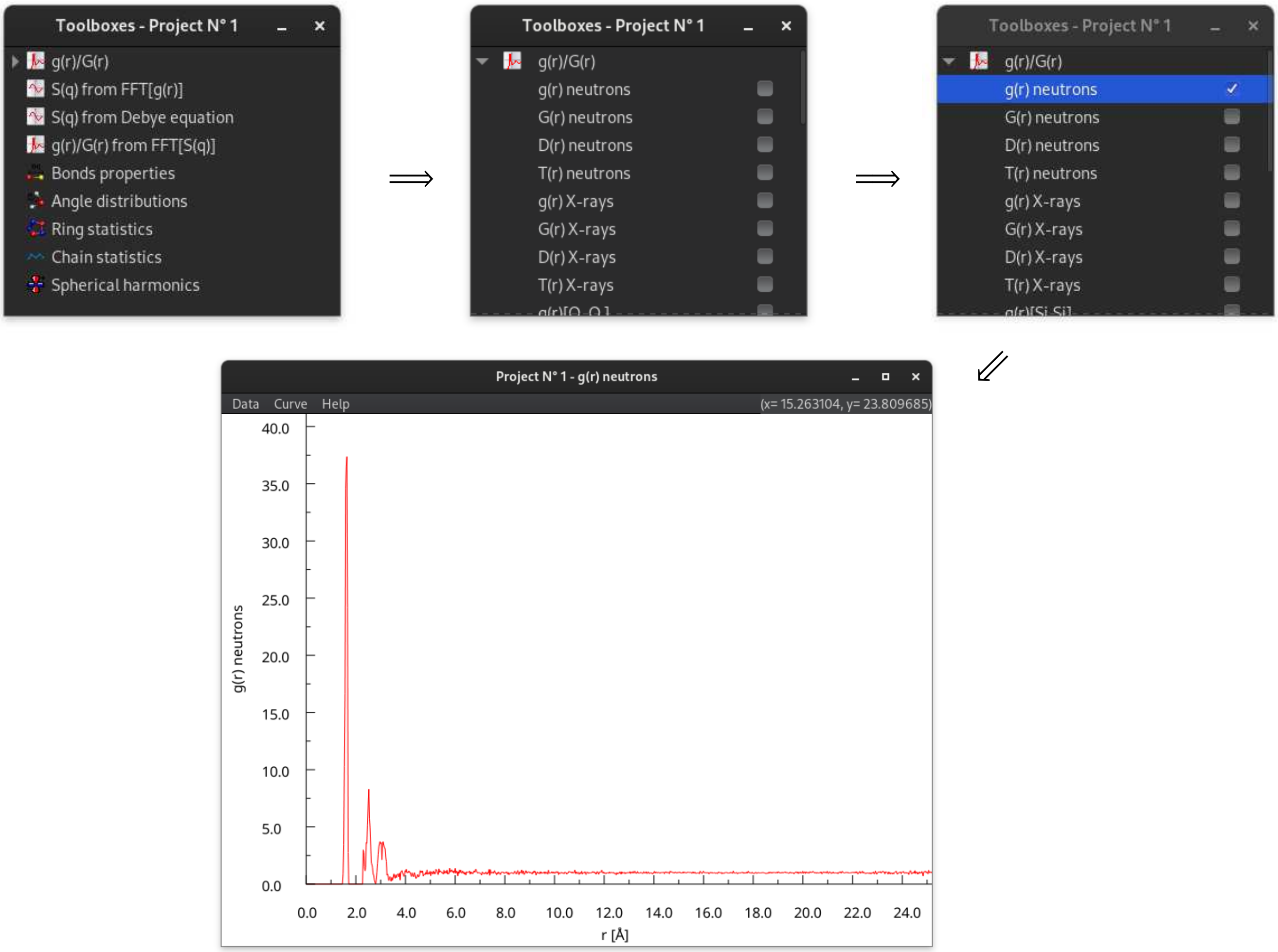
Number of δr steps 1000

D$_{max}$ = 25.216912 Å

D$_{max}$ is the maximum inter-atomic distance in the model

2.7 Visualize the results of the calculation

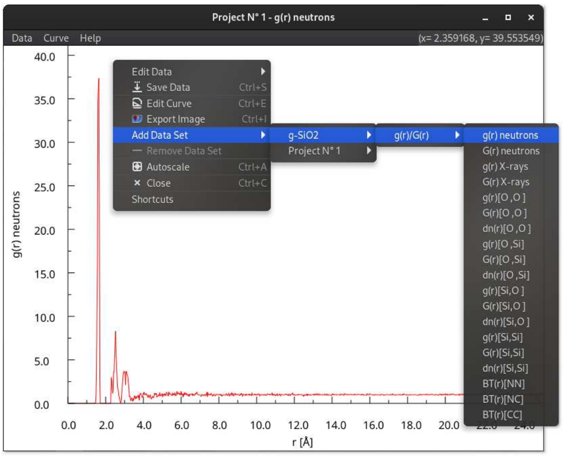
When the calculation is completed, close the dialog, and note that the content of the "`Toolboxes`" dialog is updated, the results of the calculation being available:


Toolboxes - Project N° 1
g(r)/G(r)
S(q) from FFT[g(r)]
S(q) from Debye equation
g(r)/G(r) from FFT[S(q)]
Bonds properties
Angle distributions
Ring statistics
Chain statistics
Spherical harmonics
⟹
Toolboxes - Project N° 1
g(r)/G(r)
g(r) neutrons
G(r) neutrons
D(r) neutrons
T(r) neutrons
g(r) X-rays
G(r) X-rays
D(r) X-rays
T(r) X-rays
⟹
Toolboxes - Project N° 1
g(r)/G(r)
g(r) neutrons ✓
G(r) neutrons
D(r) neutrons
T(r) neutrons
g(r) X-rays
G(r) X-rays
D(r) X-rays
T(r) X-rays
Project N° 1 - g(r) neutrons
Data
Curve
Help
(x= 15.263104, y= 23.809685)
g(r) neutrons
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
0.0
2.0
4.0
6.0
8.0
10.0
12.0
14.0
16.0
18.0
20.0
22.0
24.0
r [Å]

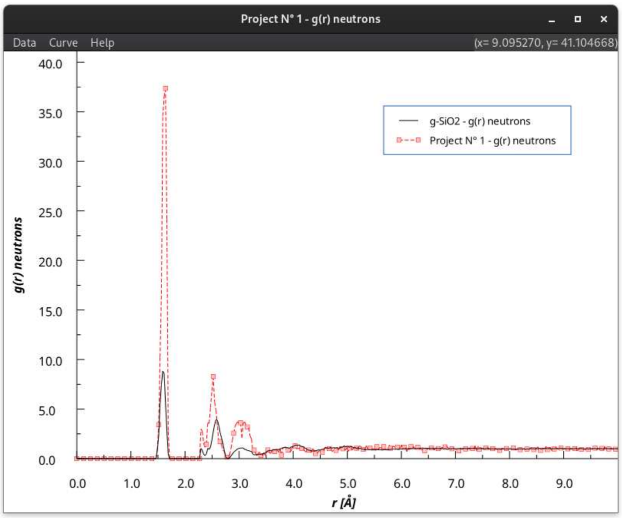
In the "`Toolboxes`" dialog open the result of the calculation to display the g(r) of the active project, in this case the new model created from the atom selection.

2.8 Add the data from the calcuation on the entire g-SiO$_2$ model

On the curve window press the mouse right click, browse the menu to "`Add Data Set -> gSiO`$_2$ `-> g(r) neutrons`" to add the corresponding data set to the representation:


Project N° 1 - g(r) neutrons
Data Curve Help
(x= 2.359168, y= 39.553549)
Edit Data
Save Data Ctrl+S
Edit Curve Ctrl+E
Export Image Ctrl+I
Add Data Set
Remove Data Set
Autoscale Ctrl+A
Close Ctrl+C
Shortcuts
g-SiO2
Project N° 1
g(r)/G(r)
g(r) neutrons
G(r) neutrons
g(r) X-rays
G(r) X-rays
g(r)[O ,O]
G(r)[O ,O]
dn(r)[O ,O]
g(r)[O ,Si]
G(r)[O ,Si]
dn(r)[O ,Si]
g(r)[Si,O]
G(r)[Si,O]
dn(r)[Si,O]
g(r)[Si,Si]
G(r)[Si,Si]
dn(r)[Si,Si]
BT(r)[NN]
BT(r)[NC]
BT(r)[CC]
g(r) neutrons
r [Å]
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
0.0 2.0 4.0 6.0 8.0 10.0 12.0 14.0 16.0 18.0 20.0 22.0 24.0

⟹

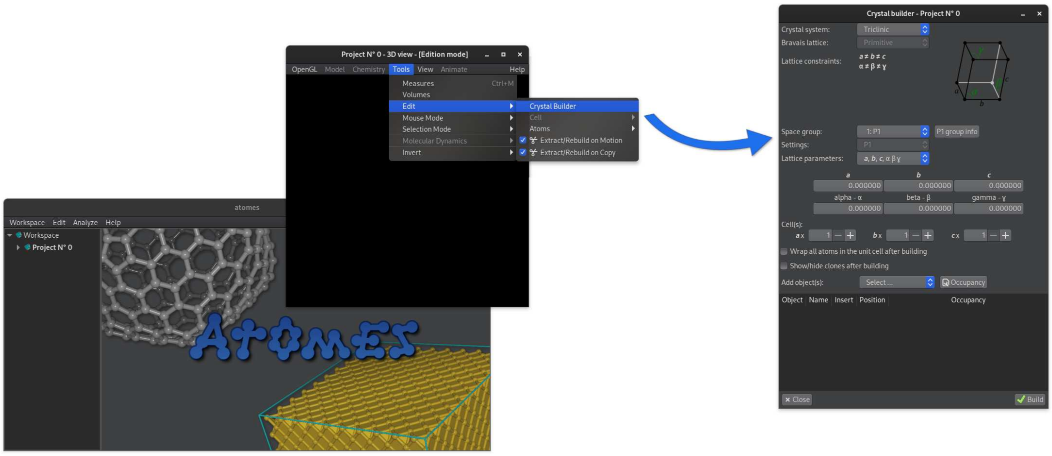

Project N° 1 - g(r) neutrons
Data Curve Help
(x= 9.095270, y= 41.104668)
g-SiO2 - g(r) neutrons
Project N° 1 - g(r) neutrons
g(r) neutrons
r [Å]
40.0
35.0
30.0
25.0
20.0
15.0
10.0
5.0
0.0
0.0 1.0 2.0 3.0 4.0 5.0 6.0 7.0 8.0 9.0

Note that projects opened in **atomes** share data. Therefore calculation results, from any model in the workspace and provided that the calculations have been performed, can be compared easily. In this example it allows to compare the g(r) for the *g*-SiO$_2$ system with a partial contribution from the atoms involved in King's rings of size 6. Comprehensive layout options are available and presentation can be clarified, each data set customized, so that the results of the analysis are quickly publication ready.

Building a crystal, then creating and passivating a surface

3.1 Create an empty project to build a crystal

Create a new empty project: "`Workspace -> Project -> New`" or press Ctrl + n , then open the crystal builder for the new, and empty, 3D window: "`Tools -> Edit -> Crystal Builder`"


atomes
Workspace
Edit
Analyze
Help
Workspace
Project N° 0
ATOMES
Project N° 0 - 3D view - [Edition mode]
OpenGL
Model
Chemistry
Tools
View
Animate
Help
Measures
Ctrl+M
Volumes
Edit
Mouse Mode
Selection Mode
Molecular Dynamics
Invert
Crystal Builder
Cell
Atoms
☑ Extract/Rebuild on Motion
☑ Extract/Rebuild on Copy
Crystal builder - Project N° 0
P1 group info
Occupancy
Object
Name
Insert
Position
Occupancy
Close
Build
a
b
c

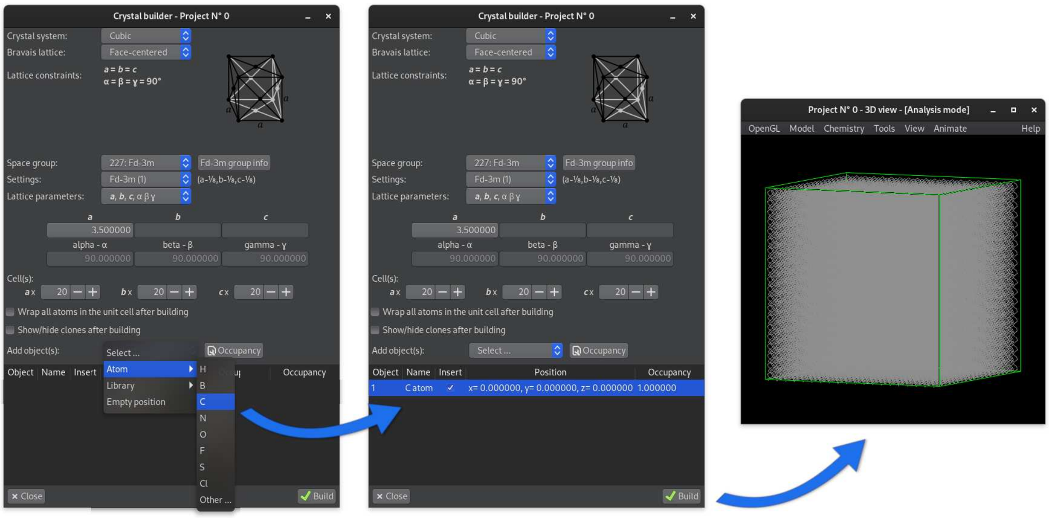
Crystal system: Triclinic
Bravais lattice: Primitive
Lattice constraints: $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma$
Space group: 1: P1
Settings: P1
Lattice parameters: $a, b, c, \alpha\ \beta\ \gamma$

a	b	c
0.000000	0.000000	0.000000
alpha - α	beta - β	gamma - γ
0.000000	0.000000	0.000000

Cell(s):
a x 1
b x 1
c x 1
☐ Wrap all atoms in the unit cell after building
☐ Show/hide clones after building
Add object(s): Select ...

3.2 Build a large diamond-like structure

Adjust parameters to selected space group and corresponding settings, in this example large diamond-like crystal: Cubic, Face-centered, space group N°227 "Fd-3m (1)" Select the object(s) to be inserted at crystalline position(s), in this example C atom(s), note that in **atomes** it is also possible to use molecular fragments inserted from the software library or from any project opened in the workspace. If needed adjust position, and / or occupancy, then remember to select the object(s) to be actually inserted when building the crystal by clicking on "Insert". Then simply click on "`Build`".


Crystal builder - Project N° 0

Crystal system: Cubic

Bravais lattice: Face-centered

Lattice constraints: $a = b = c$, $\alpha = \beta = \gamma = 90°$

Space group: 227: Fd-3m

Settings: Fd-3m (1) (a-⅛,b-⅛,c-⅛)

Lattice parameters: a, b, c, α β γ

a: 3.500000

alpha - α: 90.000000 beta - β: 90.000000 gamma - γ: 90.000000

Cell(s): a x 20 b x 20 c x 20

☐ Wrap all atoms in the unit cell after building

☐ Show/hide clones after building

Crystal builder - Project N° 0

Crystal system: Cubic

Bravais lattice: Face-centered

Lattice constraints: $a = b = c$, $\alpha = \beta = \gamma = 90°$

Space group: 227: Fd-3m

Settings: Fd-3m (1) (a-⅛,b-⅛,c-⅛)

Lattice parameters: a, b, c, α β γ

a: 3.500000

alpha - α: 90.000000 beta - β: 90.000000 gamma - γ: 90.000000

Cell(s): a x 20 b x 20 c x 20

☐ Wrap all atoms in the unit cell after building

☐ Show/hide clones after building

Object	Name	Insert	Position	Occupancy
1	C atom	✓	x= 0.000000, y= 0.000000, z= 0.000000	1.000000

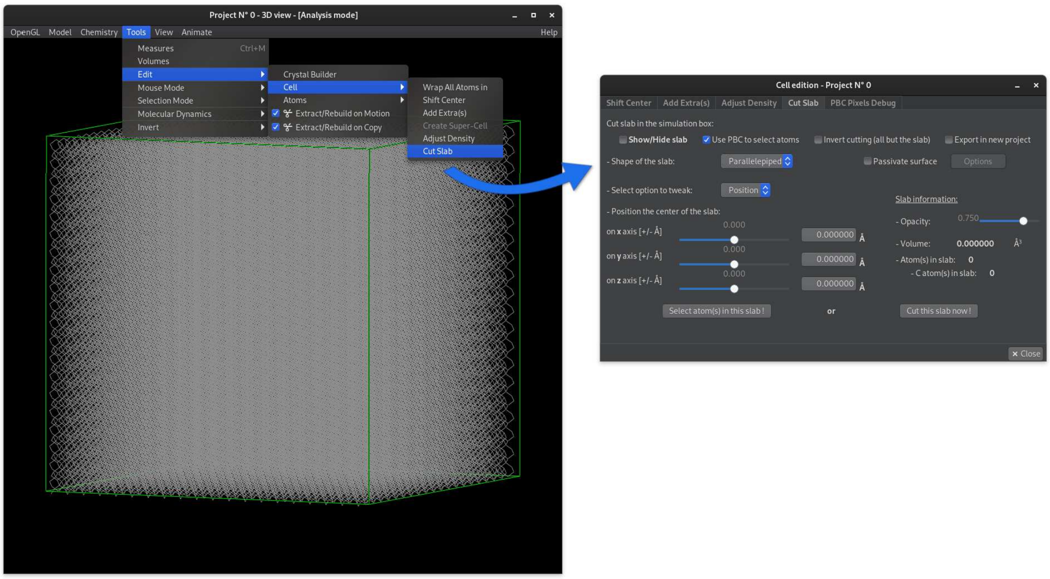
Project N° 0 - 3D view - [Analysis mode]

Fd-3m group info
Add object(s):
Select ...
Occupancy
Object
Name
Insert
Occupancy
Atom
Library
Empty position
H
B
C
N
O
F
S
Cl
Other ...
Close
Build
OpenGL
Model
Chemistry
Tools
View
Animate
Help

The 3D window is populated with the newly created structure, in this example a "20×20×20" supercell of pure diamond.

3.3 Open the surface creation utility

To create a surface in this crystalline material, open the dedicated tool: `"Tools -> Edit -> Cell -> Cut Slab"`


Project N° 0 - 3D view - [Analysis mode]
OpenGL
Model
Chemistry
Tools
View
Animate
Help
Measures Ctrl+M
Volumes
Edit
Mouse Mode
Selection Mode
Molecular Dynamics
Invert
Crystal Builder
Cell
Atoms
☑ Extract/Rebuild on Motion
☑ Extract/Rebuild on Copy
Wrap All Atoms in
Shift Center
Add Extra(s)
Create Super-Cell
Adjust Density
Cut Slab
Cell edition - Project N° 0
Shift Center
Add Extra(s)
Adjust Density
Cut Slab
PBC Pixels Debug
Options
Select atom(s) in this slab !
or
Cut this slab now !
✕ Close

Cut slab in the simulation box:

☐ **Show/Hide slab** ☑ Use PBC to select atoms ☐ Invert cutting (all but the slab) ☐ Export in new project

- Shape of the slab: Parallelepiped ☐ Passivate surface

- Select option to tweak: Position

- Position the center of the slab:

on **x** axis [+/- Å] 0.000 0.000000 Å

on **y** axis [+/- Å] 0.000 0.000000 Å

on **z** axis [+/- Å] 0.000 0.000000 Å

Slab information:

- Opacity: 0.750

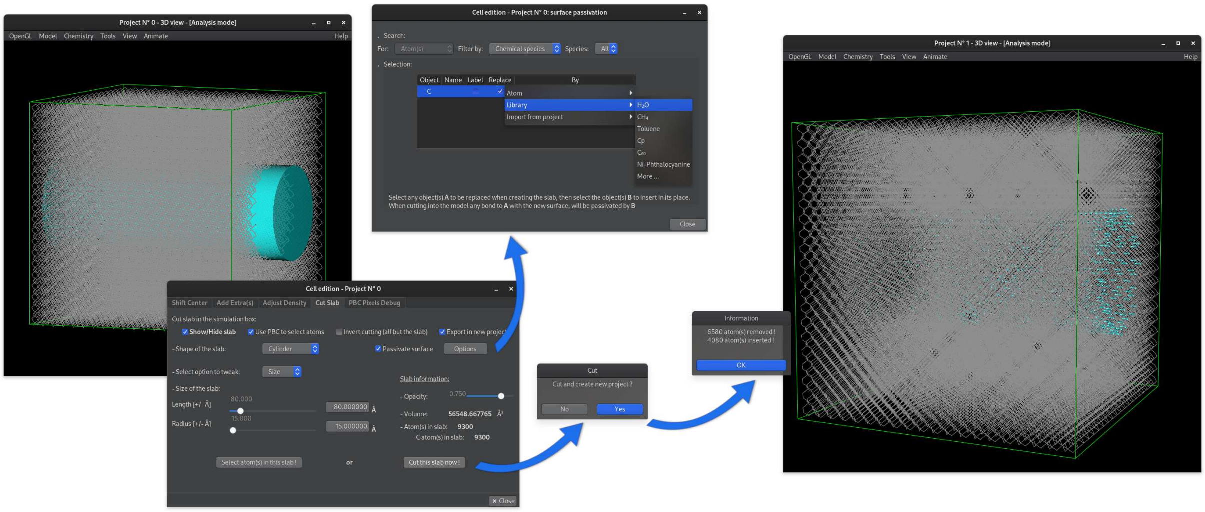
- Volume: **0.000000** Å³

- Atom(s) in slab: **0**

  - C atom(s) in slab: **0**

3.4 Prepare and cut a cylinder slab

Adjust the shape of the slab to "`Cylinder`", in the "`Size`" options adjust the cylinder length and radius to 80 Å and 15 Å respectively. You can display the slab using the "`Show/Hide slab`" interactor, also export the results of the cutting/passivating in a new project by activating the corresponding option.
Check on "`Passivate surface`" and, in the option dialog that immediately opens, and as illustrated select to passivate empty C-C bonds created when cutting the slab with water molecule.


Project N° 0 - 3D view - [Analysis mode]
OpenGL Model Chemistry Tools View Animate Help
Cell edition - Project N° 0: surface passivation
Atom
Library
Import from project
H_2O
CH_4
Toluene
Cp
C_{60}
Ni-Phthalocyanine
More ...
Close
Cell edition - Project N° 0
Shift Center
Add Extra(s)
Adjust Density
Cut Slab
PBC Pixels Debug
Options
Select atom(s) in this slab !
or
Cut this slab now !
Close
Cut
No
Yes
Information
OK
Project N° 1 - 3D view - [Analysis mode]
OpenGL Model Chemistry Tools View Animate Help

Search:
For: Atom(s) Filter by: Chemical species Species: All

Selection:

Object	Name	Label	Replace	By
C			✓	

Select any object(s) **A** to be replaced when creating the slab, then select the object(s) **B** to insert in its place.
When cutting into the model any bond to **A** with the new surface, will be passivated by **B**

Cut slab in the simulation box:
☑ Show/Hide slab ☑ Use PBC to select atoms ☐ Invert cutting (all but the slab) ☑ Export in new project
- Shape of the slab: Cylinder ☑ Passivate surface
- Select option to tweak: Size
- Size of the slab:
Length [+/- Å] 80.000 80.000000 Å
Radius [+/- Å] 15.000 15.000000 Å

Slab information:
- Opacity: 0.750
- Volume: 56548.667765 Å³
- Atom(s) in slab: 9300
- C atom(s) in slab: 9300

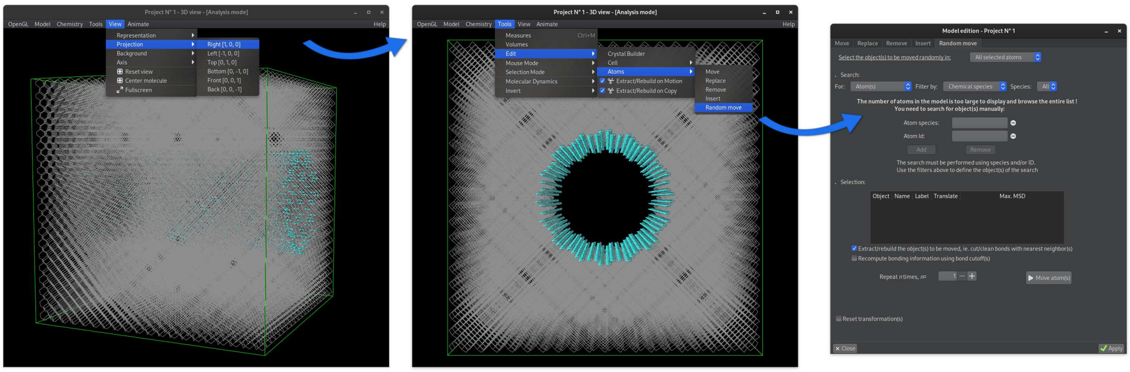
Cut and create new project ?

6580 atom(s) removed !
4080 atom(s) inserted !

Then just click on "`Cut this slab now !`" to create a new project, that will contain the new material: a C diamond cell where the atoms inside the cylinder are removed, creating a surface, and where non-bridging bonds have been passivated using H_2O molecules.

3.5 Check the model and open the "`Model Edition`" dialog

Newly inserted water molecules, under selection, appear in light blue. If you rotate to model box to face right, water molecules appear perfectly aligned. To create disorder open the "`Random Move`" tab of the "`Model Edition`" dialog: "`Tools -> Edit -> Atoms -> Random Move`"


Project N° 1 - 3D view - [Analysis mode]
OpenGL
Model
Chemistry
Tools
View
Animate
Help
Representation
Projection
Background
Axis
Reset view
Center molecule
Fullscreen
Right [1, 0, 0]
Left [-1, 0, 0]
Top [0, 1, 0]
Bottom [0, -1, 0]
Front [0, 0, 1]
Back [0, 0, -1]
Project N° 1 - 3D view - [Analysis mode]
OpenGL
Model
Chemistry
Tools
View
Animate
Help
Measures Ctrl+M
Volumes
Edit
Mouse Mode
Selection Mode
Molecular Dynamics
Invert
Crystal Builder
Cell
Atoms
☑ Extract/Rebuild on Motion
☑ Extract/Rebuild on Copy
Move
Replace
Remove
Insert
Random move
Model edition - Project N° 1
Move
Replace
Remove
Insert
Random move
Add
Remove
Object
Name
Label
Translate
Max. MSD
Move atom(s)
Close
Apply

Select the object(s) to be moved randomly in: All selected atoms

Search:

For: Atom(s) Filter by: Chemical species Species: All

The number of atoms in the model is too large to display and browse the entire list !
You need to search for object(s) manually:

Atom species:

Atom Id:

The search must be performed using species and/or ID.
Use the filters above to define the object(s) of the search

Selection:

☑ Extract/rebuild the object(s) to be moved, ie. cut/clean bonds with nearest neighbor(s)

☐ Recompute bonding information using bond cutoff(s)

Repeat *n* times, *n*= 1

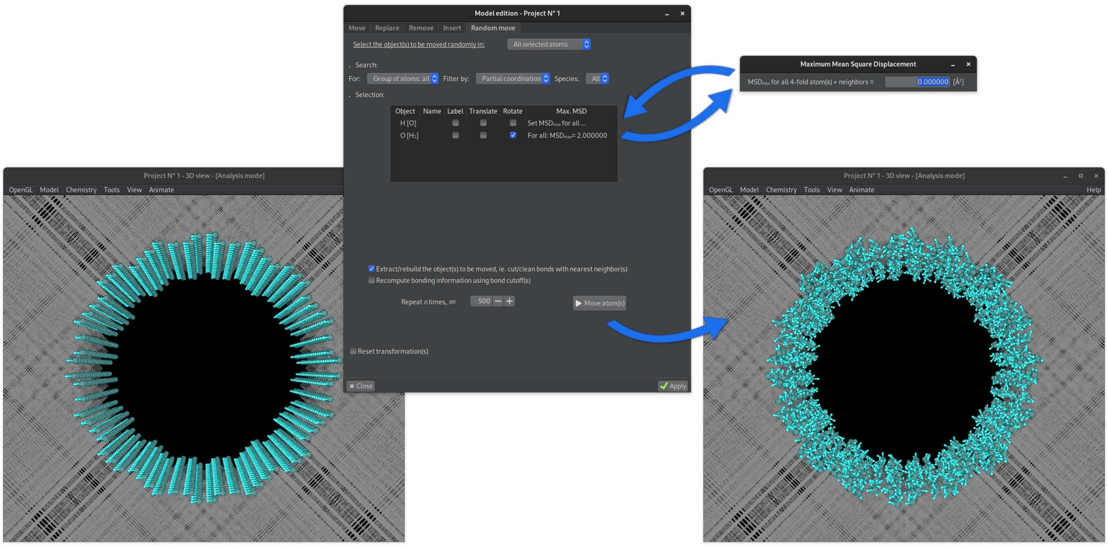
☐ Reset transformation(s)

3.6 Randomly rotate all water molecules to create disorder

This interface allows to search for, and move randomly, atom(s) or group of atom(s), selection target(s) appearing in the table bellow. Also note that, quite conveniently, "`All selected atoms`" are by default targets of the action(s) to be performed.
To work on water molecules set the search parameters as follow:

- "`For`": use "`Group of atomes: all`" to work on group of atoms, and not atom(s) individually, and to display a single interactor for all object(s) instead of a list detailed list.
- "`Filter`": use "`Partial coordination`", to display a list of partial coordination(s) matching previously set criteria.

Then selected to "`Rotate`" all "`O[H`$_2$`]`" coordination spheres, that is all water molecules, set a maximum Mean Square Displacement by adjusting the corresponding parameter, and if required specify how many times the process is to be repeated.



Model edition - Project N° 1

Select the object(s) to be moved randomly in: All selected atoms

Search:
For: Group of atoms: all Filter by: Partial coordination Species: All

Selection:

Object	Name	Label	Translate	Rotate	Max. MSD
H [O]		☐	☐	☐	Set MSD$_{max}$ for all ...
O [H$_2$]		☐	☐	☑	For all: MSD$_{max}$= 2.000000

☑ Extract/rebuild the object(s) to be moved, ie. cut/clean bonds with nearest neighbor(s)
☐ Recompute bonding information using bond cutoff(s)

Repeat *n* times, *n*= 500

☐ Reset transformation(s)

Maximum Mean Square Displacement

MSD$_{max}$ for all 4-fold atom(s) + neighbors = 0.000000 [Å^2]

Then simply click on "`Move atom(s)`" to rotate randomly and separately each water molecule in the model.

This document has been prepared using the Linux operating system and Free softwares:

The text editor	"gVim"
The GNU image manipulation program	"The Gimp"
The WYSIWYG plotting tool	"Grace"
And the document preparation system	"$\LaTeX\,2_{\varepsilon}$".