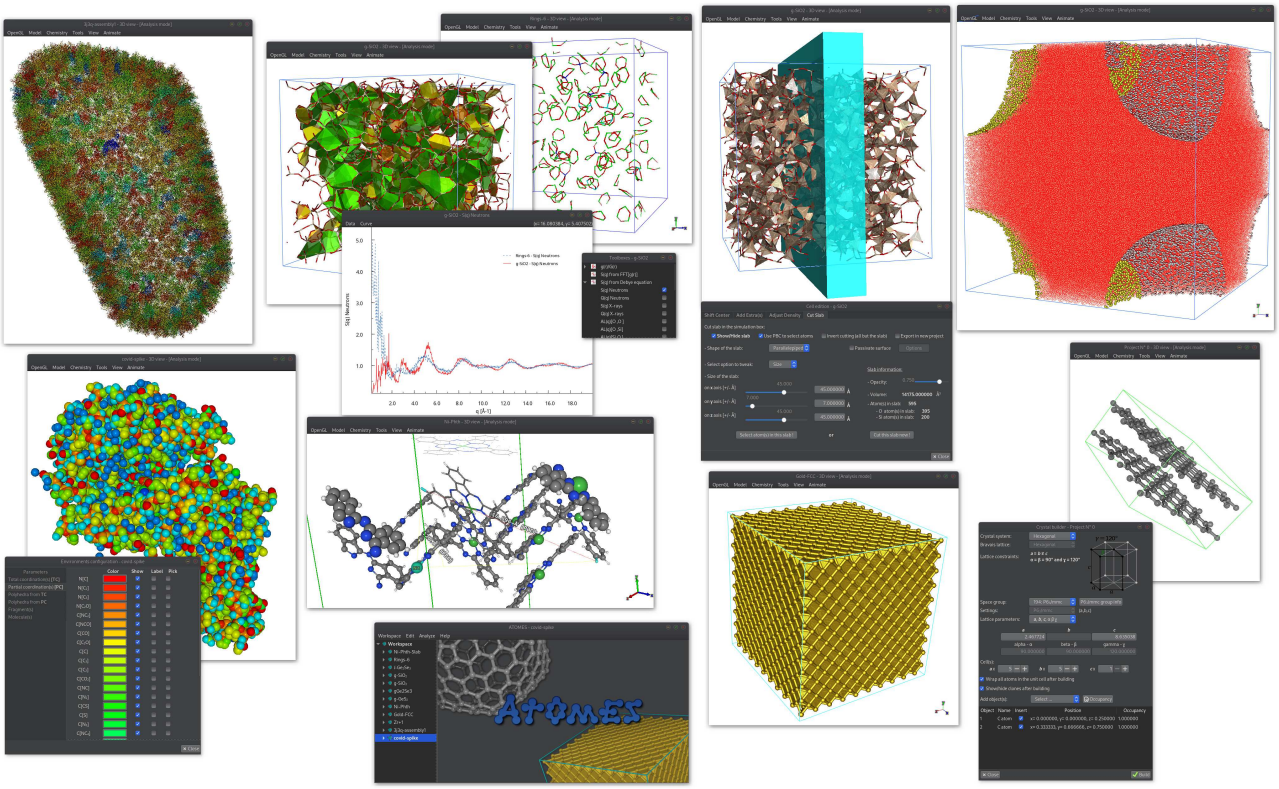
atomes

https://atomes.ipcms.fr



atomes tutorials

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Contents

Introduction

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

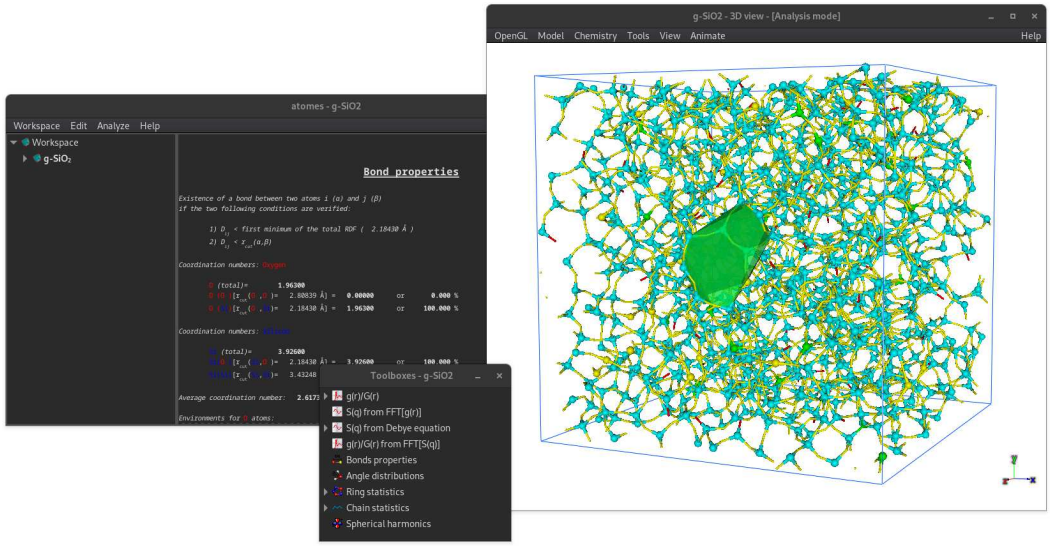
- Getting information on selected structural features: g(r) in *g*-SiO_2.
- Building a crystal, then creating and passivating a surface.

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

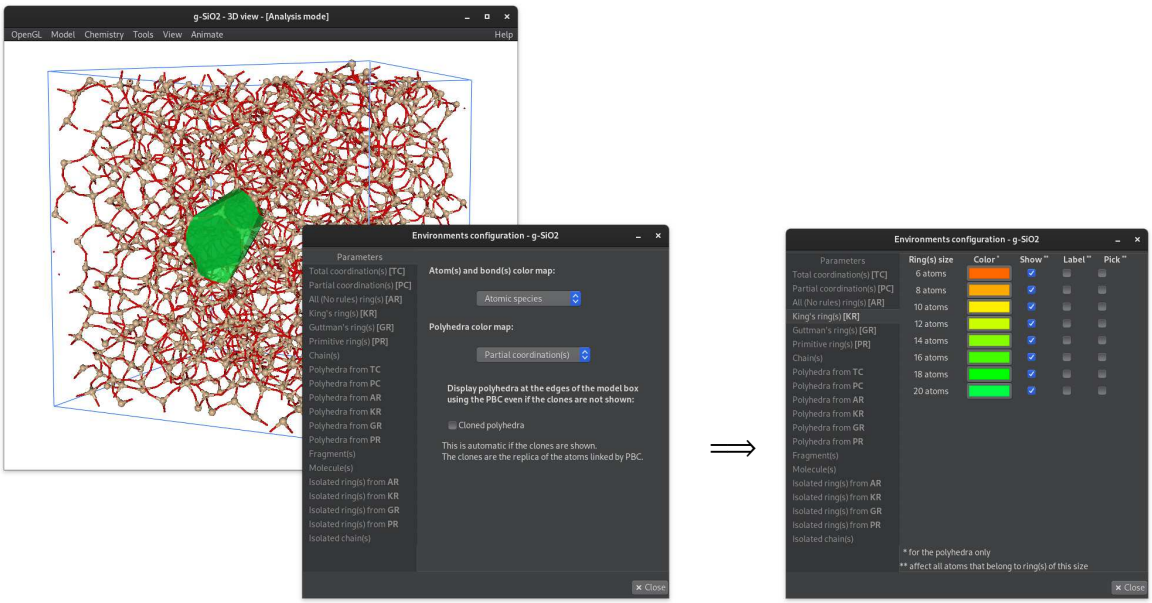
Open the **atomes** project file for the system "g-SiO_2 with ring statistics and custom color map, 3000 atoms"



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

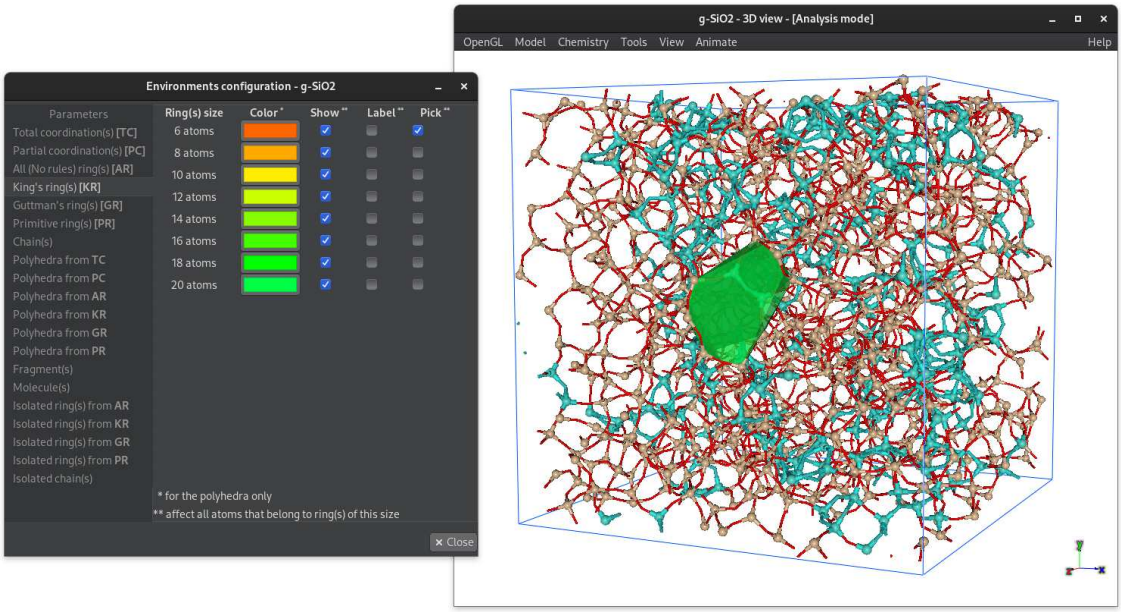
Go back to the 3D window of the g-SiO_2 model, for clarity purpose change color map to standard chemical species: from the "`OpenGL -> Color Scheme(s)`" menu, or press [a] as many times as required. Then open the "`Environments configuration`" window: from the "`Chemistry`" menu or press [Ctrl] + [e],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



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.

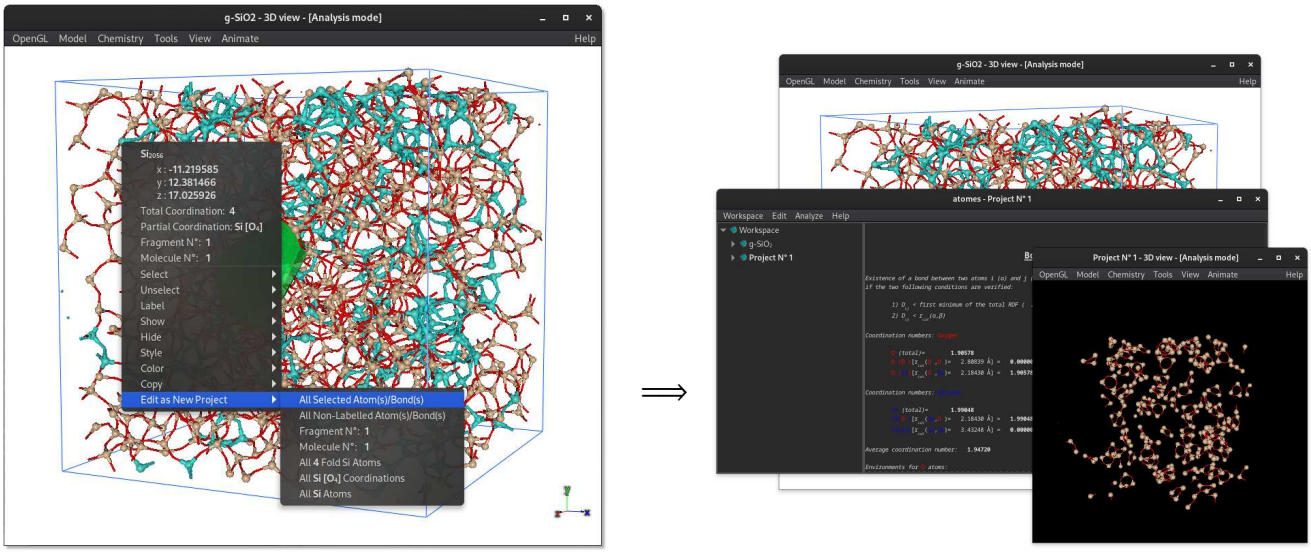
2.3 Select all atoms in ring(s) of size 6

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



2.4 Create a new model using the atom selection

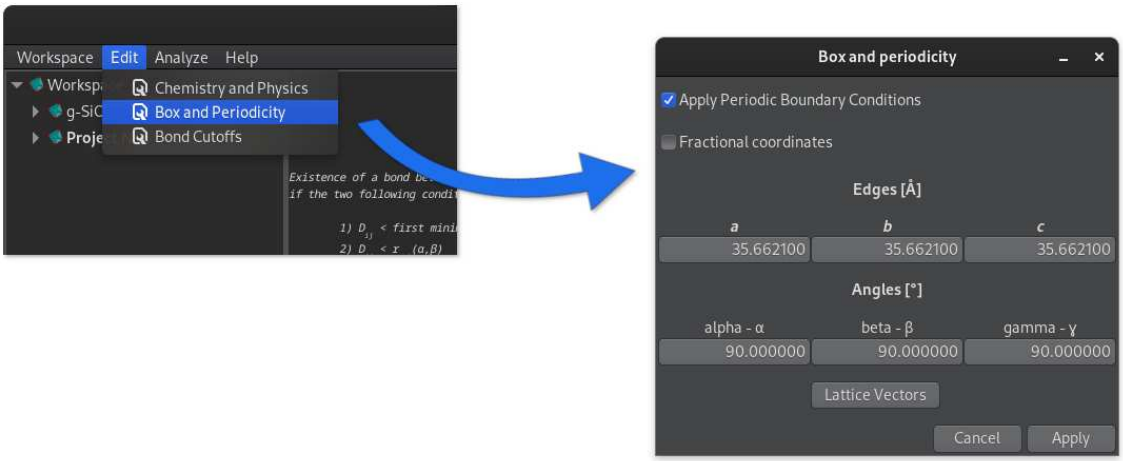
Go back to the 3D window, and mouse right click on any selected atom, then browse the contextual menu that pops up to "`Edit as New Project`", then select "`All Selected Atom(s)/Bond(s)`"



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

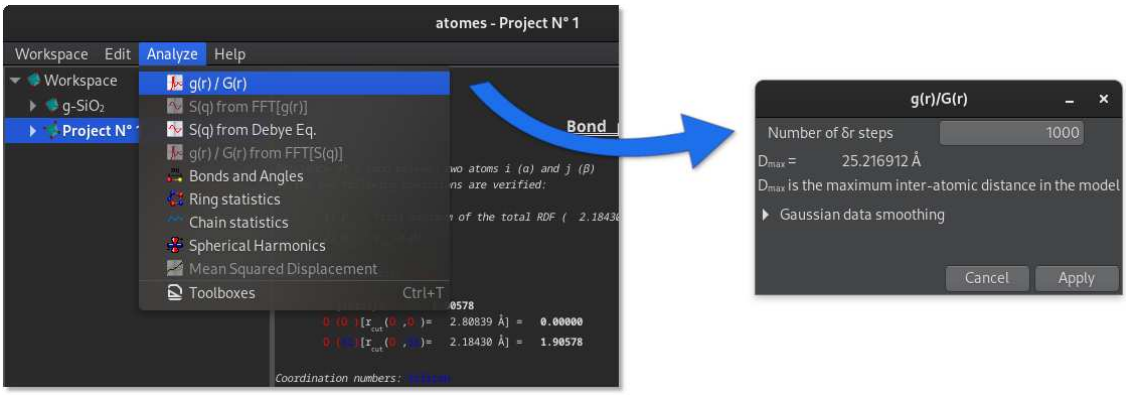
From the main interface open the "`Edit`" menu and select "`Box and Periodicity`" to reproduce the periodicity of the initial model describing properly the simulation box (a = b = c = 35.6621 Å, $\alpha = \beta = \gamma = 90$ °, and be sure to use Periodic Boundary Conditions), then apply changes.



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`".

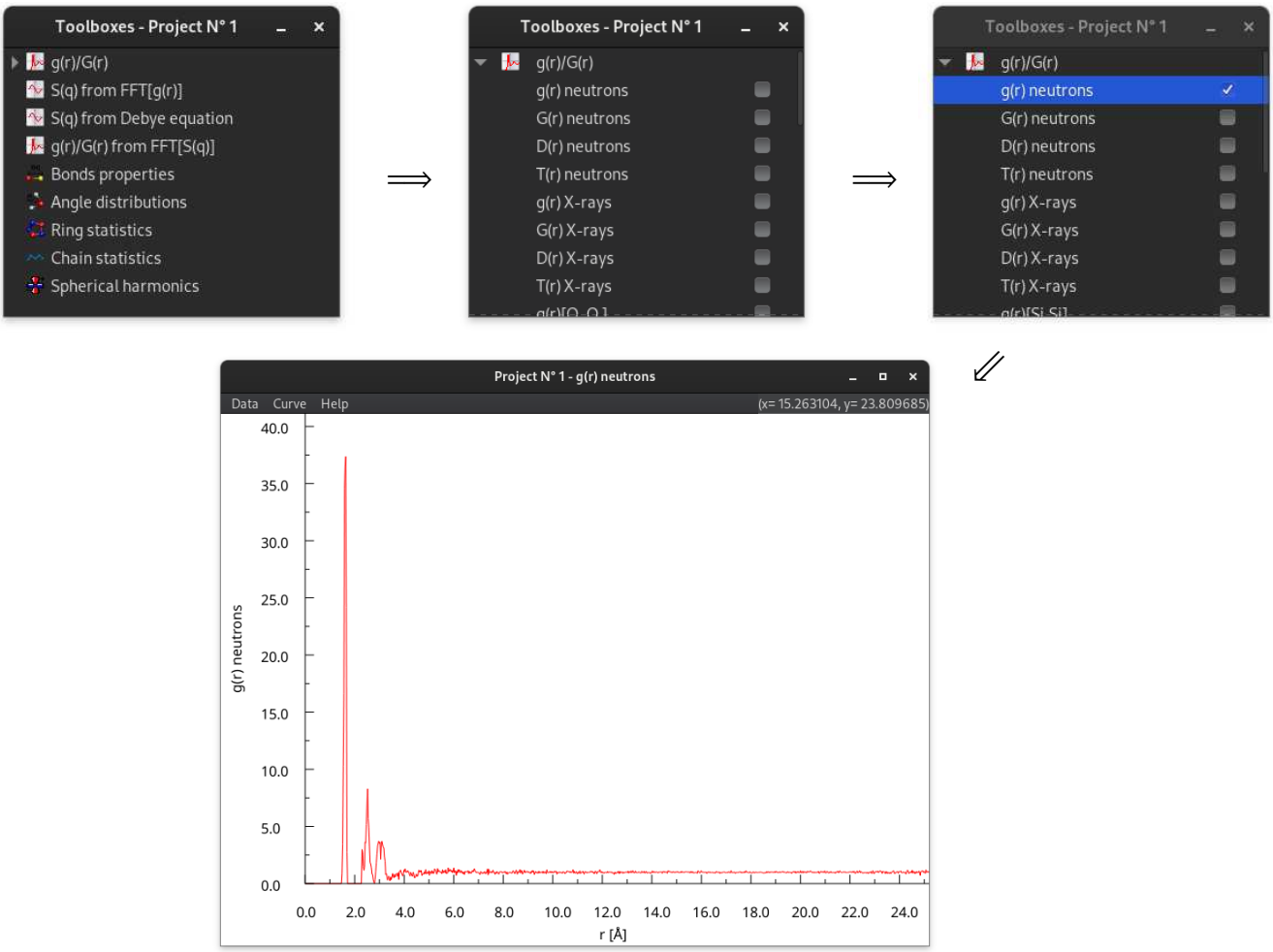
2.6 Compute the g(r) for the new model

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.



2.7 Visualize the results of the calculation

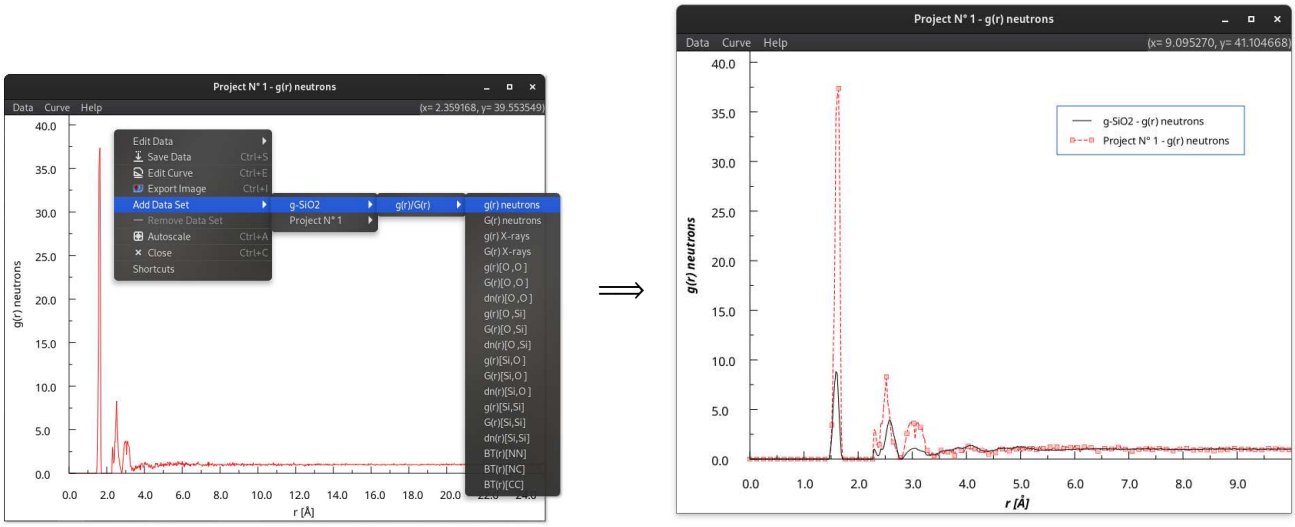
When the calculation is completed, close the dialog, and note that the content of the "`Toolboxes`" dialog is updated, the results of the calculation being available:



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 calculation data for the entire g-SiO_2 model

On the curve window press the mouse right click, browse the menu to "`Add Data Set -> gSiO2 -> g(r) neutrons`" to add the corresponding data set to the representation:

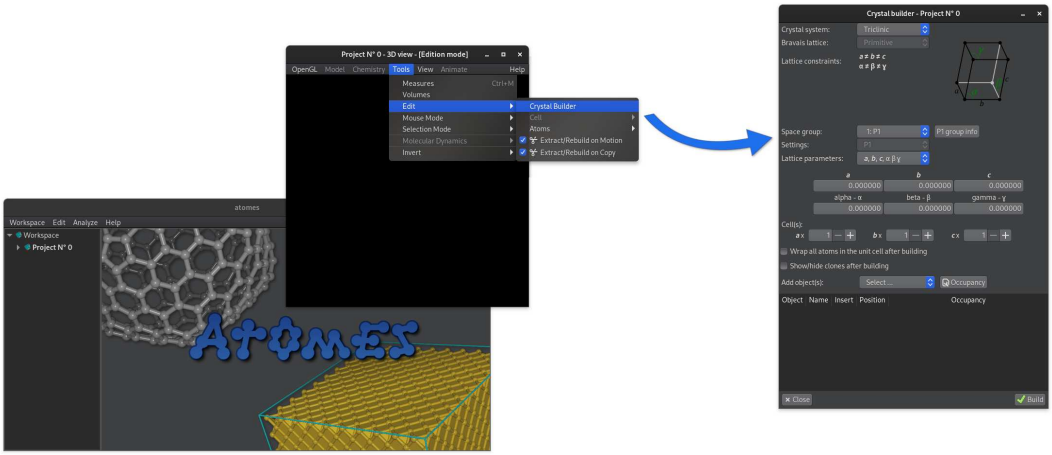


Note that projects opened in **atomes** share data. Therefore calculation results, from any model in the workspace and provided that the calculations have been performed, can be compared easily. In this example it allows to compare the g(r) for the g-SiO_2 system with a partial contribution from the 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

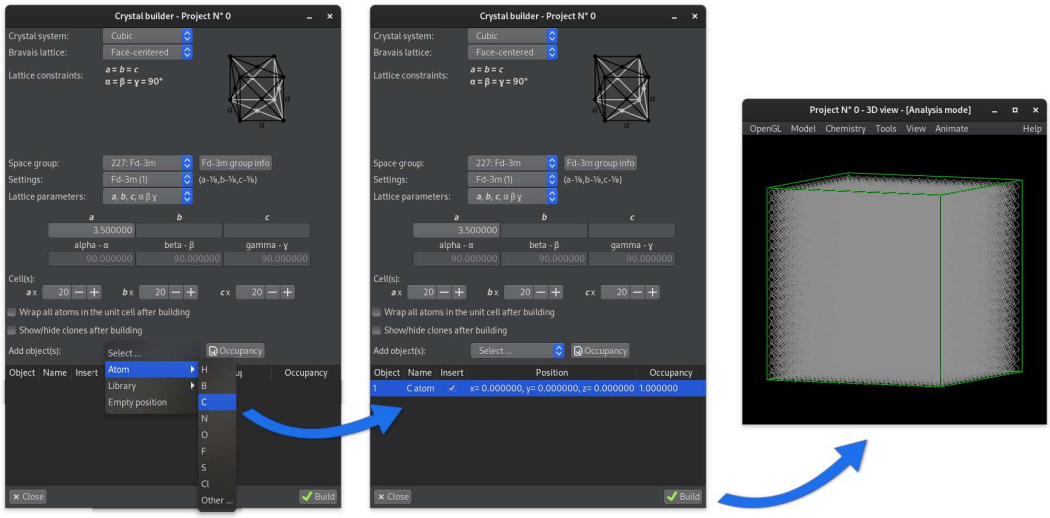
3.1 Create an empty project to build a crystal

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`"



3.2 Build a large diamond-like structure

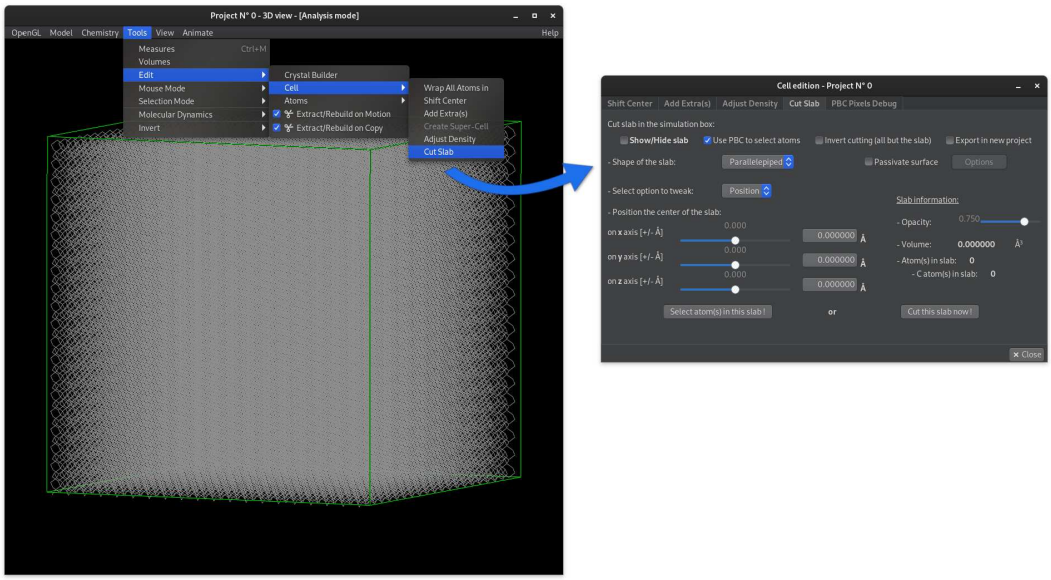
Adjust parameters to selected space group and corresponding settings, in this example large diamond-like crystal: Cubic, Face-centered, space group N°227 "Fd-3m (1)"
Select the object(s) to be inserted at crystalline position(s), in this example C atom(s), note that in **atomes** it is also possible 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`".



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

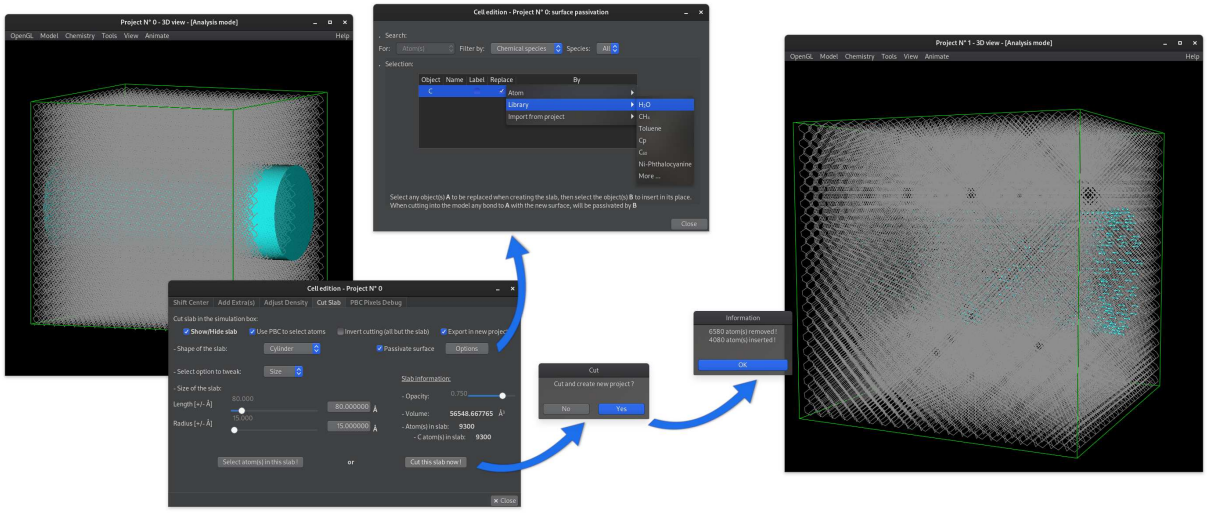
3.3 Open the surface creation utility

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



3.4 Prepare and cut a cylinder slab

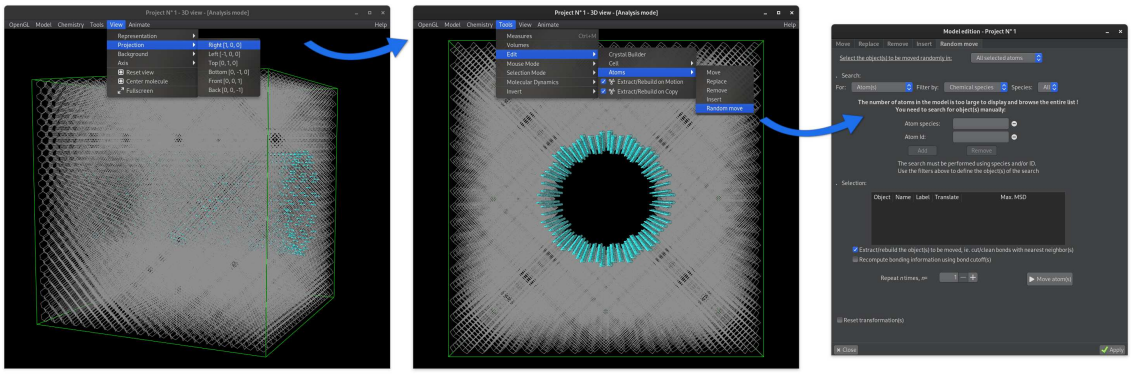
Adjust the shape of the slab to "`Cylinder`", in the "`Size`" options adjust the cylinder length and radius to 80 Å and 15 Å respectively. You can display the slab using the "`Show/Hide slab`" interactor, also export the results of the cutting/passivating in a new project by activating the corresponding 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.



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`"

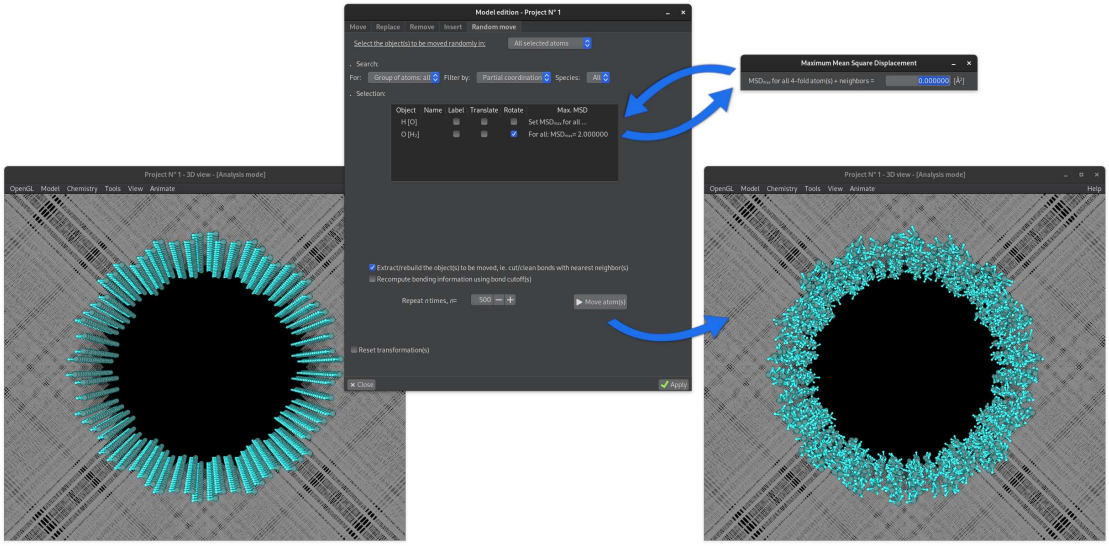


3.6 Randomly rotate all water molecules to create disorder

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[H2]`" 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.



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_ε".