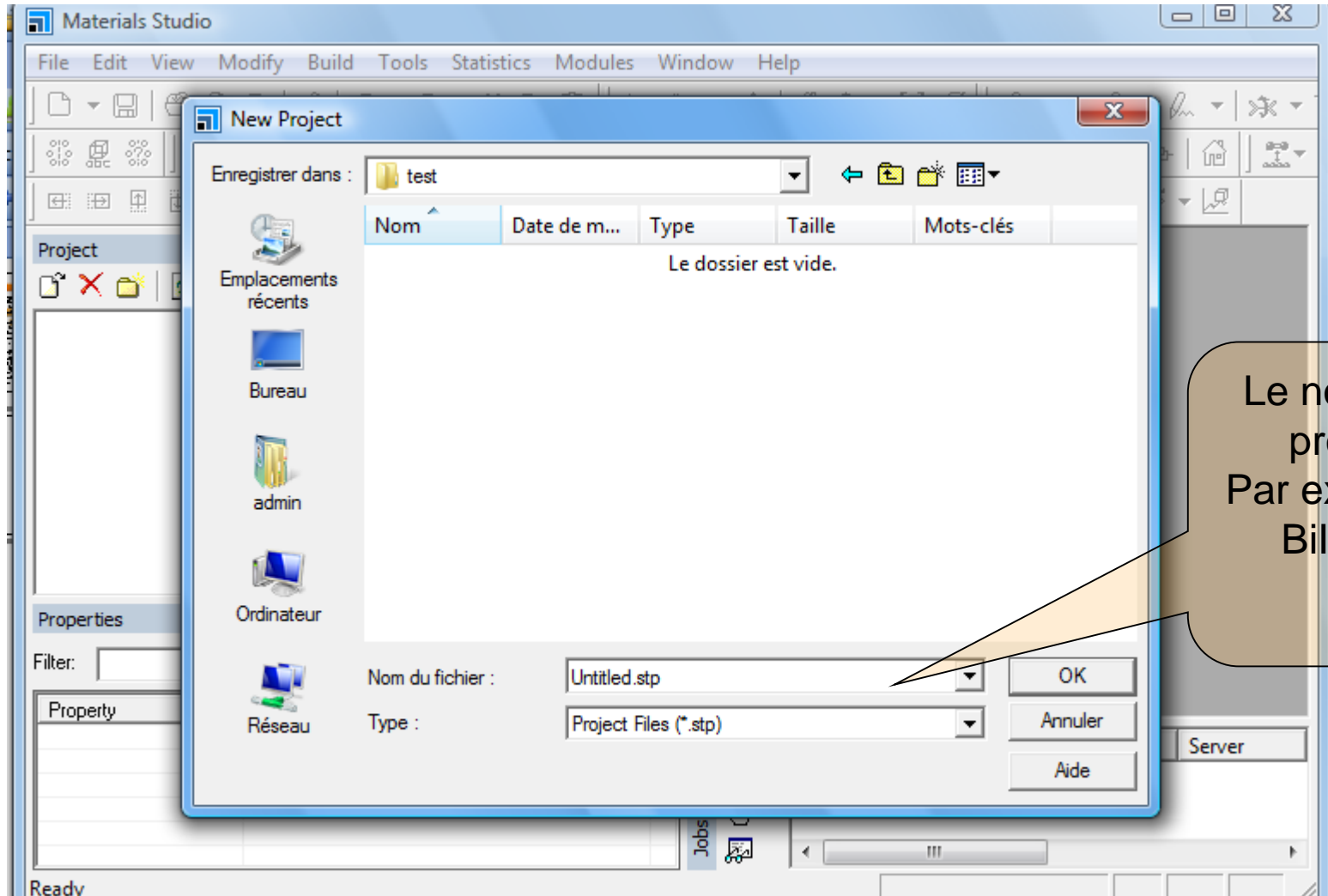


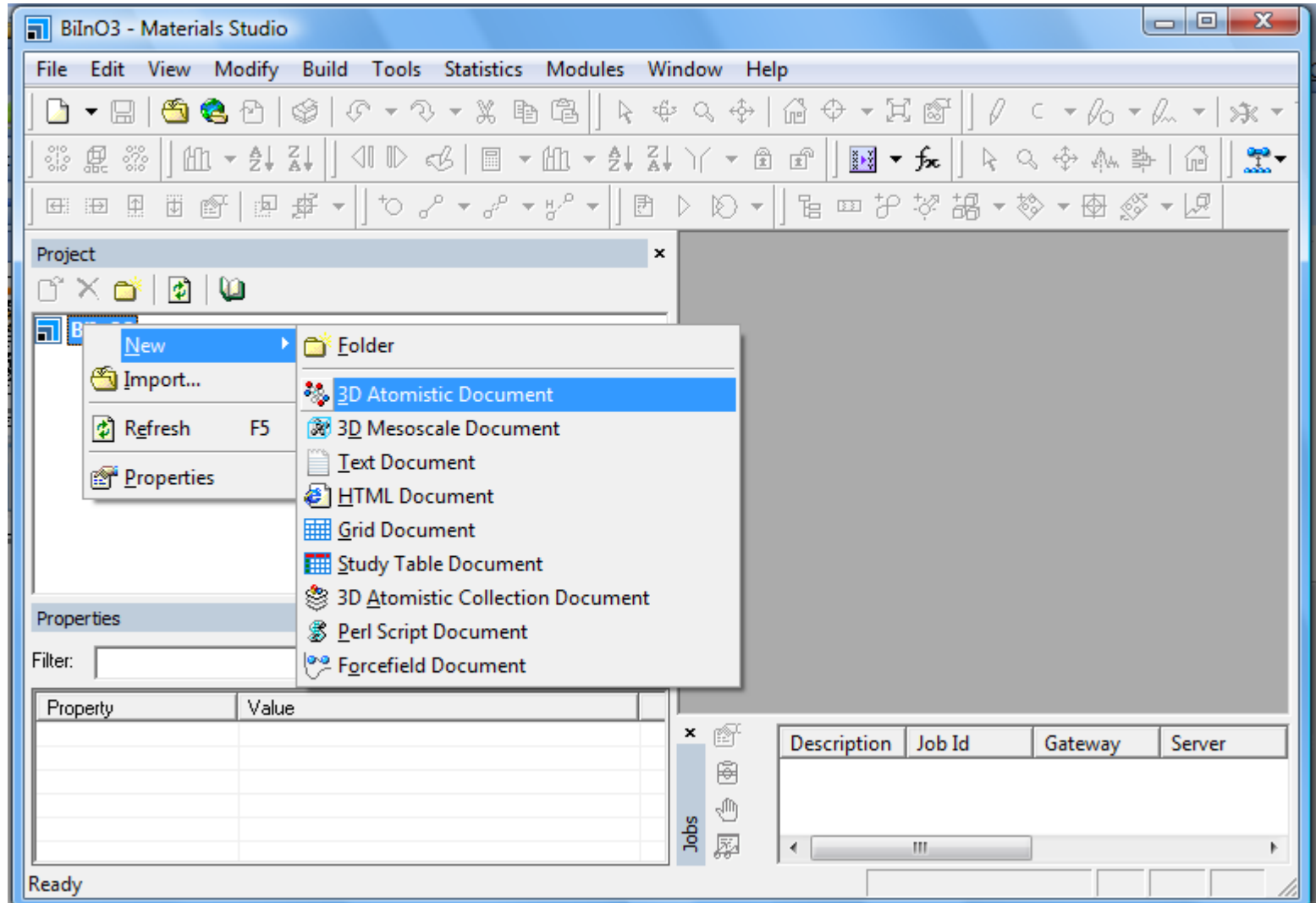
بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

انشاء برنامج الحساب
CASTEP

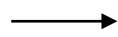
Cambridge Sequential Total Energy Package

تفاصيل برنامج الحساب وتسمية مشروع الحساب تحت اسم المركب الذي نريد حسابه

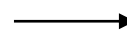




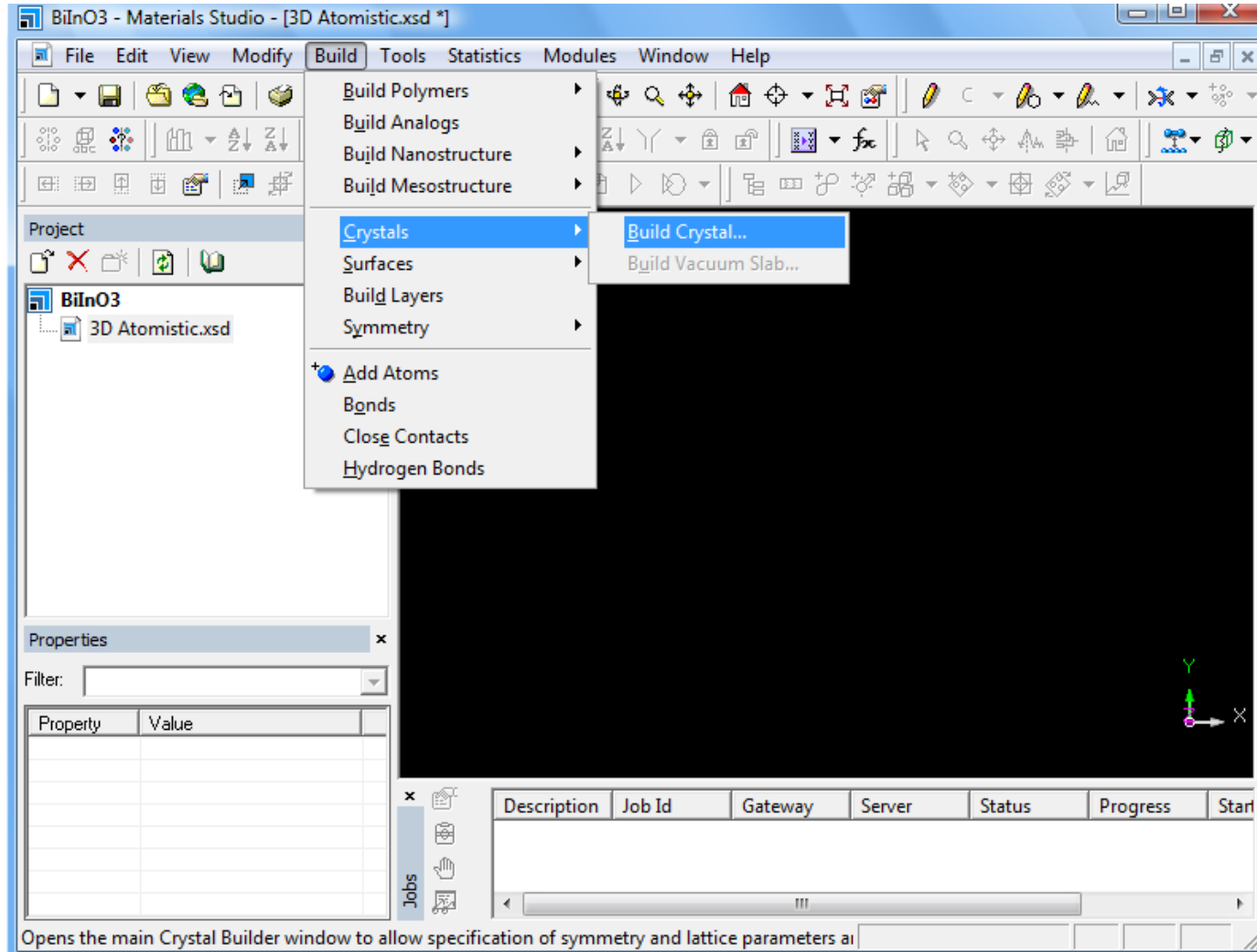
Appuyer sur Build



Crystals



Build
crystal



Build
Crystal

Space
group

Choisir le groupe d'espace adéquat
pour votre composé (MgAl_2O_4 # 227)

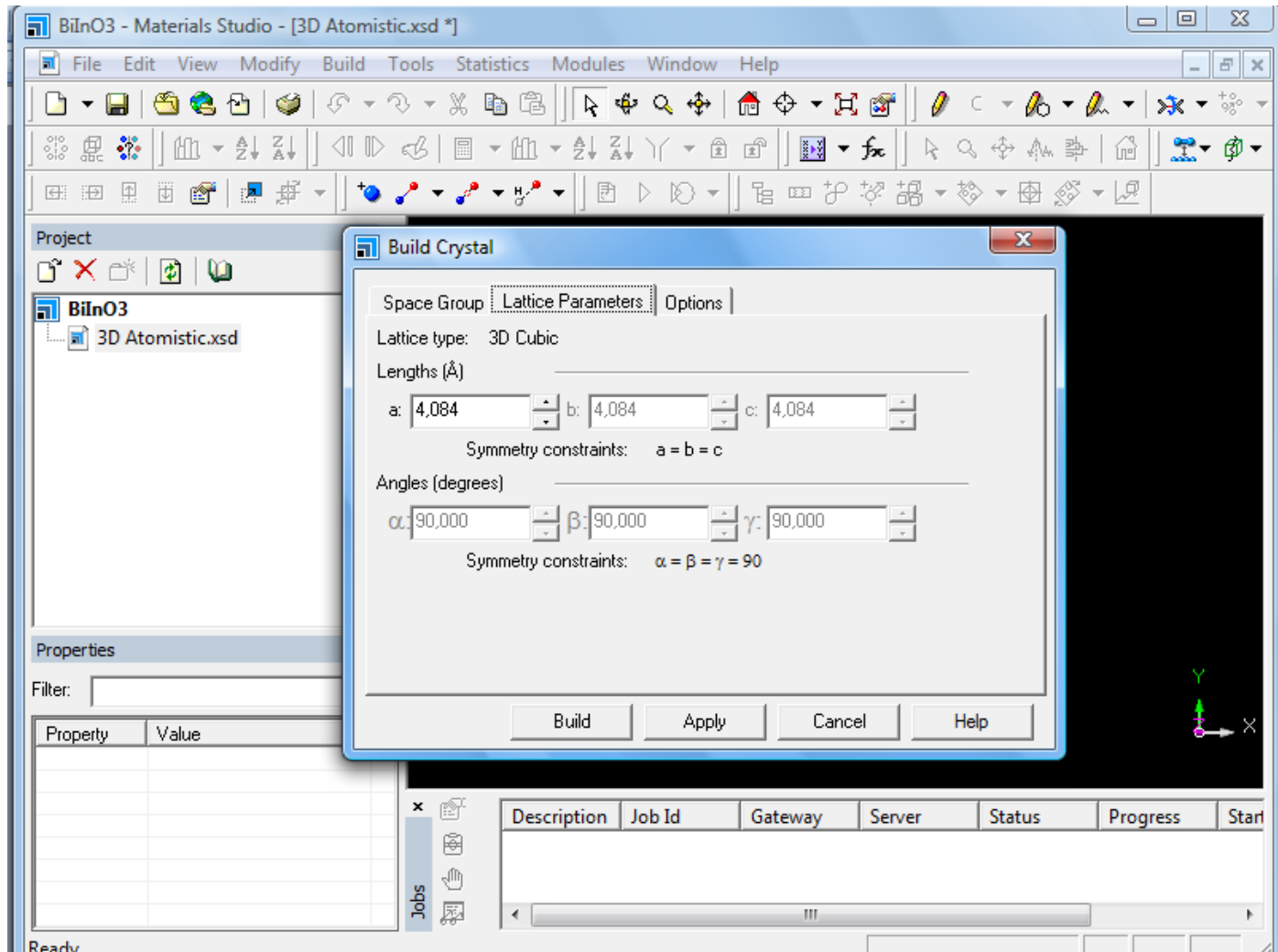
The screenshot shows the Materials Studio interface with the 'Build Crystal' dialog box open. The dialog has three tabs: 'Space Group', 'Lattice Parameters', and 'Options'. The 'Space Group' tab is active, showing a list of space groups. The 'Enter group' field is set to '221 PM-3M'. The 'List' dropdown is set to 'Cubic'. A yellow callout bubble points to the 'List' dropdown with the text 'Les sept systèmes du Bravais'. The dialog also shows a table of operators and a 'Details...' button.

Name	IT Number	Option	Long Name	Schoenflies Name	Crystal System	Crystal Class	Primitive-Centered	# of Operators
216	F-43M							
217	I-43M							
218	P-43N							
219	F-43C							
220	I-43D							
221	PM-3M		PM-3M	OH-1	Cubic	m-3m	(0,0,0)	48
222	PN-3N							
223	PM-3N							

Operator	x	y	z
1	x	y	z
2	-x	-y	z
3	-x	y	-z
4	x	-y	-z
5	z	x	y
6	z	-x	-y
7	-z	-x	y
8	-z	x	-y

Les sept
systèmes du
Bravais

إدخال ثابت الشبكة البلورية



Pour chaque type de réseau de Bravais Hexagonal, tetragonal, orthorhombique.....

إدخال احداثيات الذرات

The screenshot displays the Materials Studio interface with the 'Build' menu open. The 'Add Atoms' option is highlighted in blue. The main 3D view is currently empty, showing a coordinate system with X, Y, and Z axes. The 'Project' panel on the left shows the current project 'BiInO3' and the file '3D Atomistic.xsd'. The 'Properties' panel at the bottom left shows a table with columns for Property and Value.

Property	Value
Color	RGB(255; 255; 255)
IsVisible	
Name	
Style	

Jobs

Description	Job Id	Gateway	Server	Status	Progress	Start
-------------	--------	---------	--------	--------	----------	-------

Opens the window to allow insertion of new atoms into the structure

The screenshot displays the Materials Studio interface for a BiInO₃ project. Three 'Add Atoms' dialog boxes are open, each with 'Atoms' and 'Options' tabs. The background shows a 3D model of the crystal structure with atoms labeled B, O, and A.

Left Dialog (Bi):

- Element: Bi
- Name: Bi
- Oxidation State: 0
- Occupancy: 1,0
- Temperature Factors: None, Isotropic, Anisotropic
- Coordinates: a: 0,000, b: 0,000, c: 0,000

Middle Dialog (In):

- Element: In
- Name: [empty]
- Oxidation State: 0
- Occupancy: 1,0
- Temperature Factors: None, Isotropic, Anisotropic
- Coordinates: a: 0,500, b: 0,500, c: 0,500

Right Dialog (O):

- Element: O
- Name: O
- Oxidation State: 0
- Occupancy: 1,0
- Temperature Factors: None, Isotropic, Anisotropic
- Coordinates: a: 0,500, b: 0,500, c: 0,000

Clique droite → Display style → pour rendre les atomes sous forme sphérique

The screenshot shows the Materials Studio interface for a project named 'BiInO3'. A right-click context menu is open over a 3D model of the crystal structure, with the 'Display Style' option selected. The menu includes options for Cut (Ctrl+X), Copy (Ctrl+C), Paste (Ctrl+V), Delete, Display Style, Display Options, Lighting, Label, and Lattice Parameters. The 3D view shows a unit cell with axes labeled A, B, and C, and a coordinate system with X, Y, and Z axes. The Properties panel on the left shows the filter set to 'Atom' and a table of properties for the selected atom.

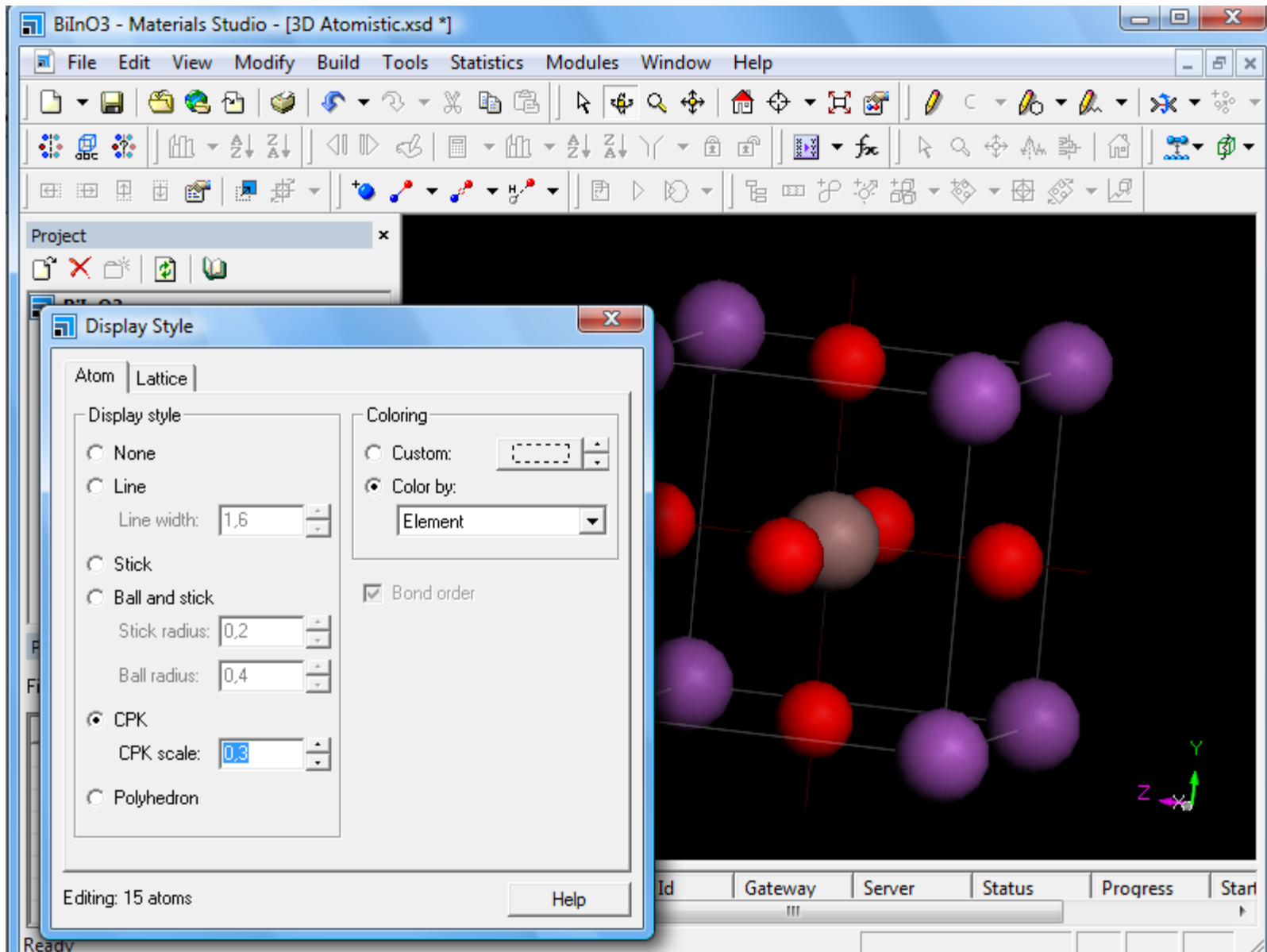
Property	Value
Charge	0,000000
Composition	
ElementNa...	
ElementSy...	
ForcefieldT...	
FormalChar...	
FormalSpin	0
FormalSpin...	Undefined

Job queue table:

Description	Job Id	Gateway	Server	Status	Progress	Start

Opens the Display Style window

Display style → CPK ou Poyhedron ou bien Ball and Stick → en même temps vous pouvez choisir les options pour Lattice.



Pour nommer les atomes ou bien une tache voulue → clique droite → Label

The screenshot shows the Materials Studio interface with a 3D model of BiInO3. A context menu is open over the model, listing options: Cut (Ctrl+X), Copy (Ctrl+C), Paste (Ctrl+V), Delete, Display Style, Display Options, Lighting, Label (highlighted), and Lattice Parameters. The Project panel on the left shows the file '3D Atomistic.xsd'. The Properties panel at the bottom left is filtered to 'Atom' and shows a table of properties.

Property	Value
Charge	0,000000
Composition	
ElementNa...	
ElementSy...	
ForcefieldT...	
FormalChar...	
FormalSpin	0
FormalSpin...	Undefined

Job x

Description	Job Id	Gateway	Server	Status	Progress	Start

Opens the Label window

Plusieurs propriétés affichées soit ce qui concerne « Atom » ou bien « Bond »

The screenshot displays the Materials Studio interface for a BiInO3 model. A 'Label' dialog box is open, showing the following configuration:

- Object type: Atom
- Font: Helvetica, size 12
- Color: (empty)
- Custom text: (empty)
- Properties list: Charge, Color, Composition, ElementName, **ElementSymbol**, ForcefieldType, FormalCharge, FormalSpin, FormalSpinDirection, FormalSpinState
- Buttons: Apply, Remove, Remove All, Help

The background shows a 3D ball-and-stick model of the BiInO3 crystal structure. The atoms are labeled: Bi (purple), In (grey), and O (red). The 'Properties' panel at the bottom left shows the following data:

Property	Value
Charge	0,000000
Composition	
ElementNa...	
ElementSy...	
ForcefieldT...	
FormalChar...	
FormalSpin	0
FormalSpin...	Undefined

كيفية استعمال البرنامج الحسابي
le code CASTEP.

Modules → CASTEP → Calculation

The screenshot shows the Materials Studio interface with the 'Modules' menu open. The 'CASTEP' option is selected, and its sub-menu is displayed, showing 'Calculation' as the active choice. The background features a 3D ball-and-stick model of a BiInO3 crystal structure with Bi atoms in purple, In atoms in grey, and O atoms in red. The interface includes a Project pane on the left showing 'BiInO3' and '3D Atomistic.xsd', a Properties pane at the bottom left with a table of atom properties, and a Job Queue table at the bottom.

Property	Value
Charge	0,000000
Composition	
ElementNa...	
ElementSy...	
ForcefieldT...	
FormalChar...	
FormalSpin	0
FormalSpin...	Undefined

Description	Job Id	Gateway	Server	Status	Progress	Start

Opens the CASTEP Calculation tool

Task —————> geometry optimization —————> Minimizer —————> coucher optimize cell

The screenshot displays the Materials Studio interface for a BiInO3 project. Two dialog boxes are open:

- CASTEP Calculation:** Shows the 'Task' set to 'Geometry Optimization' and 'Quality' set to 'Ultra-fine'. The 'Functional' is 'GGA' with 'PBE' selected. It includes checkboxes for 'Spin polarized' (unchecked) and 'Use LDA+U' (unchecked), and a checked option for 'Use formal spin as initial'. Spin and charge values are set to 0.
- CASTEP Geometry Optimization:** Shows the 'Minimizer' tab. It lists convergence criteria: Quality (Ultra-fine), Energy (5.0e-6 eV/atom), Max. force (0.01 eV/Å), Max. stress (0.02 GPa), and Max. displacement (5.0e-4 Å). It also shows 'Max. iterations' set to 100, 'Optimize cell' checked, 'Cell optimization' set to 'Fixed Basis Quality', and 'Compressibility' set to 'Hard'.

Arrows indicate the flow from the 'More...' button in the first dialog to the 'Minimizer' tab in the second, and from the 'Optimize cell' checkbox in the second dialog to the 'coucher optimize cell' text in the header.

Task → geometry optimization → more et choisir l'algorithme voulu

The screenshot displays the Materials Studio interface for a BiInO3 project. Two dialog boxes are open:

- CASTEP Calculation:** Shows the 'Task' set to 'Geometry Optimization' and 'Quality' set to 'Ultra-fine'. The 'Functional' is set to 'GGA' and 'PBE'. There are checkboxes for 'Spin polarized' (unchecked) and 'Use formal spin as initial' (checked). The 'Initial spin' and 'Charge' are both set to 0.
- CASTEP Geometry Optimization:** Shows the 'Minimizer' tab with the 'Algorithm' set to 'BFGS'. There are checkboxes for 'Use delocalized internals' (unchecked) and 'Auto-update time step' (unchecked). The 'Damping algorithm' is set to 'Independent', the 'Damping coefficient recalculation frequency' is 30, and the 'Wavefunction extrapolation' is '1st W'. The 'Time step' is 1.0 fs.

Arrows point from the 'More...' button in the first dialog to the 'Algorithm' dropdown in the second dialog, and from the 'BFGS' option in the dropdown to the 'BFGS' label in the dialog title bar.

Cette tache nous permet de introduire la valeur du pression hydrostatique

The image shows the Materials Studio interface with two dialog boxes open. The 'CASTEP Calculation' dialog is in the foreground, showing 'Task: Geometry Optimization' and 'Functional: GGA'. The 'CASTEP Geometry Optimization' dialog is also open, with the 'Stress' tab selected. It displays a table for 'External stress (GPa)' with columns for x, y, and z, and a field for 'Equivalent hydrostatic pressure' set to 0.0. A yellow callout bubble points to the hydrostatic pressure field with the text: 'La pression Est un tenseur Injecter directement La valeur voulue ici'.

	x	y	z
x:	0,0	0,0	0,0
y:	0,0	0,0	0,0
z:	0,0	0,0	0,0

Equivalent hydrostatic pressure: 0,0

BiInO3 - Materials Studio - [3D Atomistic.xsd *]

File Edit View Modify Build Tools Statistics Modules Window Help

Project

BiInO3

3D Atomistic.xsd

Properties

Filter: Atom

Property	Value
Charge	0,000000
Composition	
ElementNa...	
ElementSy...	
ForcefieldT...	
FormalChar...	
FormalSpin	0
FormalSpin...	Undefined

CASTEP Calculation

Setup Electronic Properties Job Control

Energy cutoff: Ultra-fine 380,0 eV

SCF tolerance: Ultra-fine

k-point set: Fine 6x6x6

Pseudopotentials: Ultrasoft

Pseudopotential representation: Ultrasoft

Use core hole

More...

Run Files... Help

Description Job Id Gateway Server Status Progress Start

Pseudo-potential

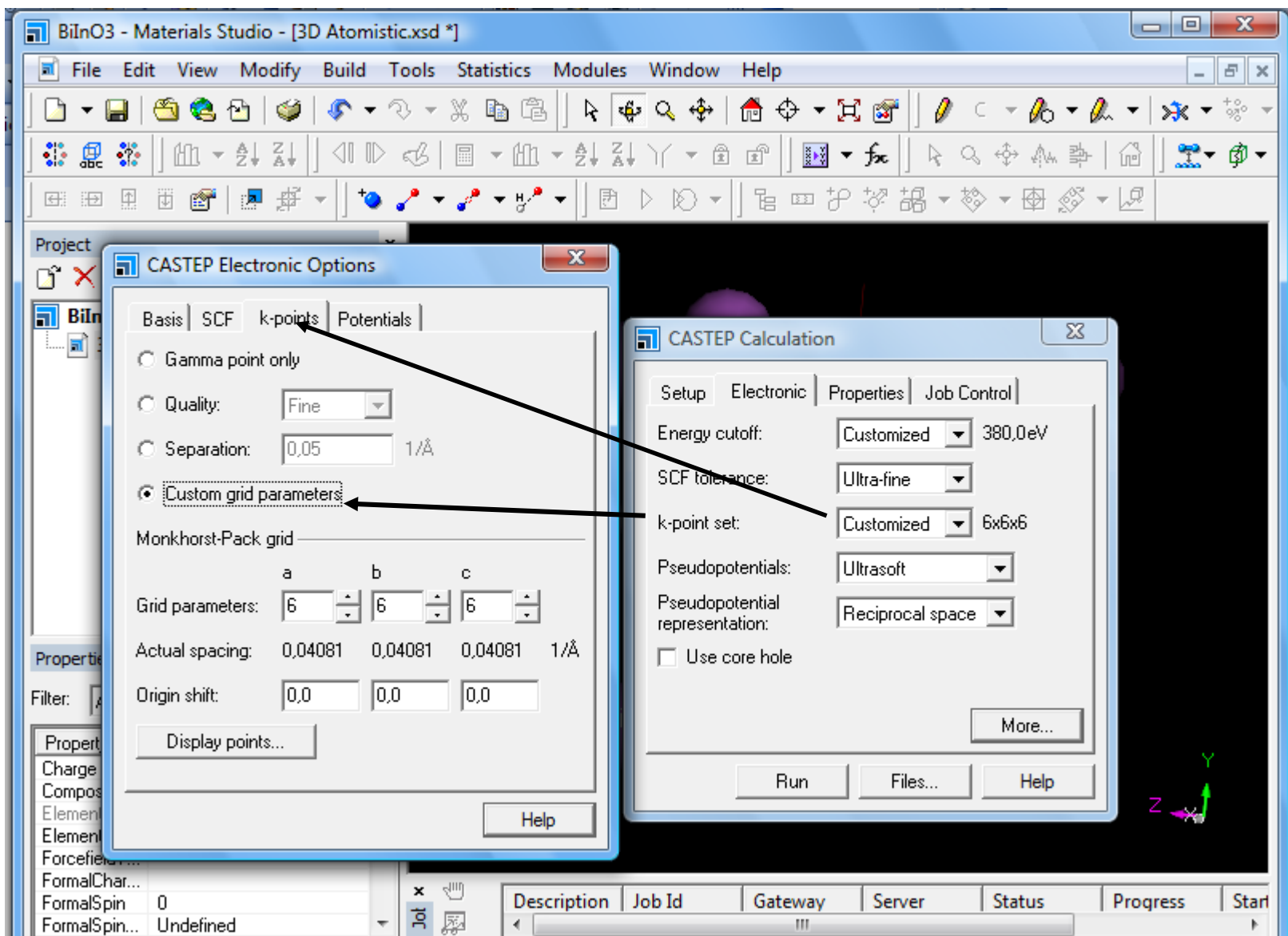
Pour des résultats d'haute performances personnaliser quelques paramètres
« Energy cut-off » « *K*-points » selon le cas

The screenshot displays the Materials Studio interface for a BiInO3 project. Two dialog boxes are open:

- CASTEP Electronic Options:** The 'Basis' tab is selected. The 'Use custom energy cut-off' checkbox is checked, with the value set to 380,0 eV. The 'Derived grid' is set to 'Precise'. The 'Divisions' are set to 30 for a, b, and c axes. The 'Apply finite basis set correction' is set to 'Smart', and the 'Correction mode' is 'Automatic'. The 'Numerical differentiation using' is set to 3 points, and the 'Energy derivative w.r.t. cutoff' is 0,0 eV.
- CASTEP Calculation:** The 'Electronic' tab is selected. The 'Energy cutoff' is set to 'Customized' at 380,0 eV. The 'SCF tolerance' is 'Ultra-fine', the 'k-point set' is 'Fine' (6x6x6), and the 'Pseudopotentials' are 'Ultrasoft'. The 'Pseudopotential representation' is 'Reciprocal space'. The 'Use core hole' checkbox is unchecked.

An arrow points from the '380,0 eV' input field in the 'CASTEP Electronic Options' dialog to the '380,0 eV' value in the 'CASTEP Calculation' dialog, illustrating the transfer of the energy cutoff parameter.

Description	Job Id	Gateway	Server	Status	Progress	Start
		!!!				



BiInO3 - Materials Studio - [3D Atomistic.xsd *]

File Edit View Modify Build Tools Statistics Modules Window Help

Project

CASTEP Electronic Options

Basis SCF k-points Potentials

Gamma point only
 Quality: Fine
 Separation: 0,05 1/Å
 Custom grid parameters

Monkhorst-Pack grid

	a	b	c	
Grid parameters:	6	6	6	
Actual spacing:	0,04081	0,04081	0,04081	1/Å
Origin shift:	0,0	0,0	0,0	

Display points...

Help

CASTEP Calculation

Setup Electronic Properties Job Control

Energy cutoff: Customized 380,0eV
 SCF tolerance: Ultra-fine
 k-point set: Customized 6x6x6
 Pseudopotentials: Ultrasoft
 Pseudopotential representation: Reciprocal space
 Use core hole

Monkhorst-Pack mesh

There are 10 irreducible k-points

0,41667	0,41667	0,41667
0,41667	0,41667	0,25000
0,41667	0,41667	0,08333
0,41667	0,25000	0,25000
0,41667	0,25000	0,08333
0,41667	0,08333	0,08333

Appuyer sur « Run » pour demarer la procédure du calcul

Faire associer tous les processeurs de votre machine pour accélérer le calcul.

The screenshot displays the Materials Studio interface with the CASTEP Calculation dialog box open. The dialog is set to the 'Job Control' tab. The 'Gateway location' is set to 'My Computer'. The 'Queue' is empty. The 'Job description' is empty, and the 'Automatic' checkbox is checked. The 'Run in parallel on' option is set to 2 of 2 processors. The 'Runtime optimization' is set to 'Default'. The 'Return complete check file' checkbox is unchecked. The 'Run' button is highlighted with a yellow callout box. The background shows a 3D model of a BiInO3 crystal structure with Bi atoms in purple and O atoms in red.

Property	Value
Charge	0,000000
Composition	
ElementNa...	
ElementSy...	
ForcefieldT...	
FormalChar...	
FormalSpin	0
FormalSpin...	Undefined

Description	Job Id	Gateway	Server	Status	Progress	Start

Materials Studio - [3D Atomistic.xsd *]

File Edit View Modify Build Tools Statistics Modules Window Help

Project

BiInO3

- 3D Atomistic CASTEP GeomOpt
 - 3D Atomistic - Calculation
 - 3D Atomistic.xsd

Properties

Filter: All

Property	Value
Name	
Style	

Jobs

Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...
<input checked="" type="checkbox"/> 3D Ato...	X6GRUL	localhost...	CASTEP	running		02/04/201...	.\3D Ato...

Ready

FR 10:56

Le programme en état de calcul

The screenshot shows the Materials Studio interface. A 'Job Completed' dialog box is open, displaying the following information:

- Job: [X6RUL] - 3D Atomistic CASTEP GeomOpt
- Program: CASTEP
- Gateway: My Computer
- Status: successfully-completed

The dialog box has an 'OK' button with a checkmark next to it. A yellow callout box points to this button with the text: "Étape du calcul est terminée, cliquer sur « OK »".

The background terminal window shows the following output:

```
PC-de-mounir
31 2013

SS TTTT EEEEE PPPP
T E P P
T EEE PPPP
T E P
CCC A A SSS T EEEEE P

welcome to Materials Studio CASTEP version 4.4
Ab Initio Total Energy Program

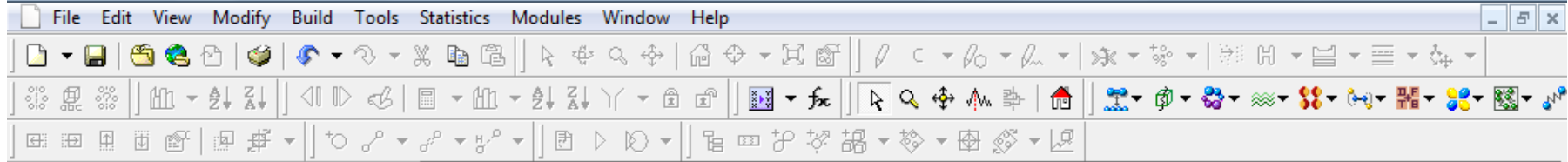
Authors:
M. Segall, M. Probert, C. Pickard, P. Hasnip,
S. Clark, K. Refson, M. Payne

Contributors:
P. Lindan, P. Haynes, J. White, V. Milman,
N. Govind, M. Gibson, P. Tulip, V. Cocula,
B. Montanari, D. Quigley, M. Glover,
L. Bernasconi, A. Perlov, M. Plummer

Copyright (c) 2000 - 2008
```

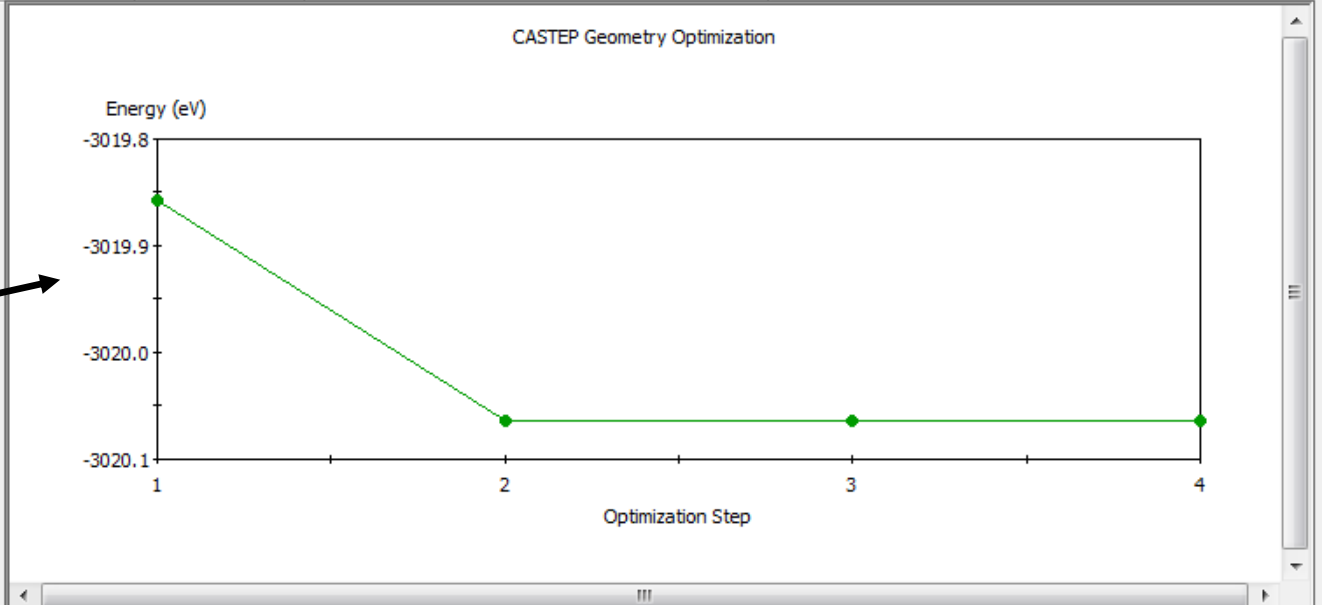
The interface also includes a 'Properties' panel on the left and a 'Jobs' table at the bottom.

Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...



Project

- BiInO3
 - 3D Atomistic CASTEP GeomOpt
 - 3D Atomistic - Calculation
 - 3D Atomistic.xsd
 - Status.txt
 - 3D Atomistic Energies.xcd
 - 3D Atomistic Convergence.xcd
 - 3D Atomistic.xtd
 - 3D Atomistic.param
 - 3D Atomistic.castep
 - 3D Atomistic.xsd

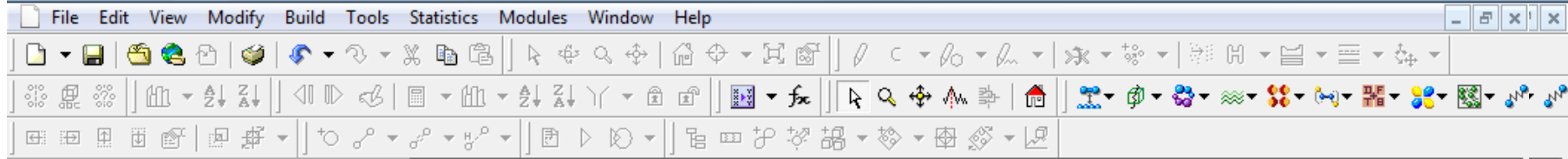


Properties

Filter:

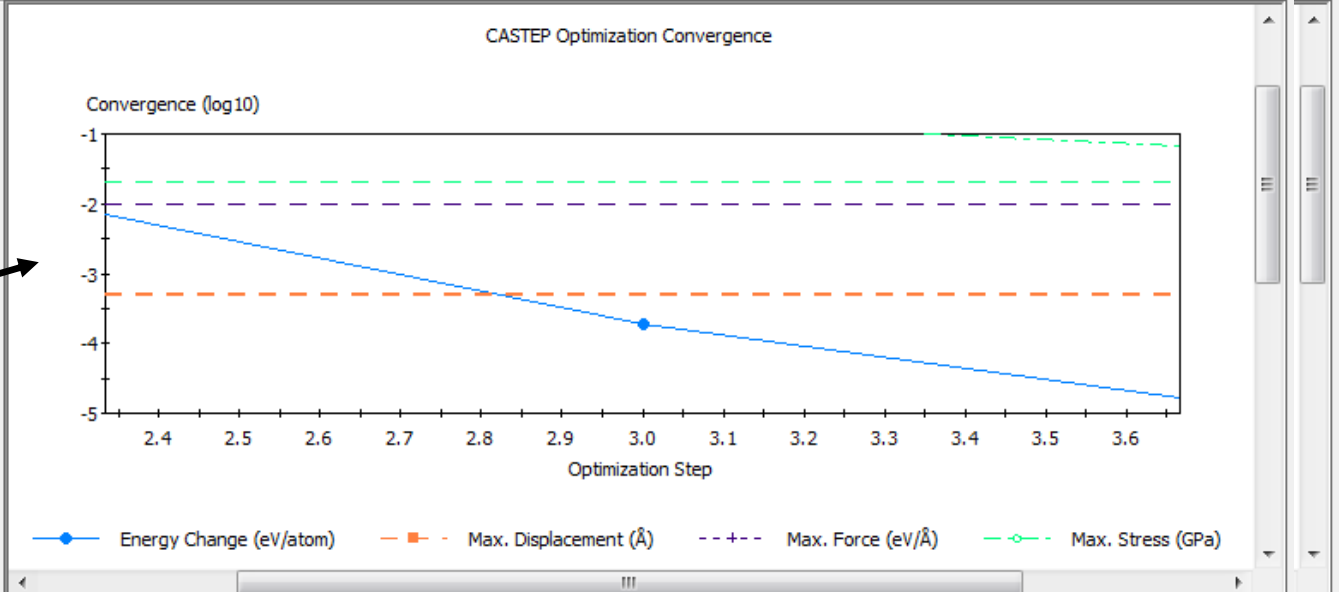
Property	Value

Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...



Project

- BiInO3
 - 3D Atomistic CASTEP GeomOpt
 - 3D Atomistic - Calculation
 - 3D Atomistic.xsd
 - Status.txt
 - 3D Atomistic Energies.xcd
 - 3D Atomistic Convergence.xcd
 - 3D Atomistic.xtd
 - 3D Atomistic.param
 - 3D Atomistic.castep
 - 3D Atomistic.xsd



Properties

Filter:

Property	Value

Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...

Calcul des propriétés électronique et optique

Tache est active sur
« Properties »

The screenshot displays the Materials Studio interface for a BiInO3 project. The main window shows a 3D ball-and-stick model of the crystal structure. A 'CASTEP Calculation' dialog box is open, with the 'Properties' tab selected. The 'Task' dropdown is set to 'Properties'. Other settings include 'Quality: Customized', 'Functional: GGA PBE', and 'Initial spin: 0'. The 'Properties' window is also open, showing a table with columns for 'Property' and 'Value'. At the bottom, a 'Jobs' table is visible with columns: Description, Job Id, Gateway, Server, Status, Progress, Start Time, and Results Fo... The Windows taskbar at the bottom shows the system clock at 11:19.

Property	Value
Name	
Style	

Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...
-------------	--------	---------	--------	--------	----------	------------	---------------

Coucher les propriétés à
calculer
« Properties »

The screenshot shows the Materials Studio interface with the following components:

- Project Panel:** Shows a project named "BiInO3" with a sub-project "3D Atomistic CASTEP GeomOpt". Under this sub-project, there is a folder "3D Atomistic - Calculation" containing files like "3D Atomistic.xsd", "Status.txt", "3D Atomistic Energies.xcd", "3D Atomistic Convergence.xcd", "3D Atomistic.xtd", "3D Atomistic.param", and "3D Atomistic.castep".
- CASTEP Calculation Dialog:** Has tabs for "Setup", "Electronic", "Properties", and "Job Control". The "Properties" tab is active, showing a list of properties to calculate:
 - Band structure
 - Core level spectroscopy
 - Density of states
 - Electron density difference
 - Electron localization function
 - NMRBelow the list, "Band structure" is expanded to show "Empty bands: 20" and "k-point set: Ultra-fine". There is a "More..." button and "Run", "Files...", and "Help" buttons at the bottom.
- CASTEP Band Structure Options Dialog:** Shows the "k-point path" table:

Sym	From	To	Sym	Div
X	0,500 0,000 0,000	0,500 0,500 0,500	R	21
R	0,500 0,500 0,500	0,500 0,500 0,000	M	15
M	0,500 0,500 0,000	0,000 0,000 0,000	G	21
G	0,000 0,000 0,000	0,500 0,500 0,500	R	26

Below the table are navigation buttons (back, forward, etc.) and a "Reset" button. At the bottom, there is a checkbox "Use separate XC functional for band structure calculation" (unchecked), "Functional:" dropdowns set to "GGA" and "PBE", and "Band energy tolerance:" set to "1,0e-5 eV". "OK", "Cancel", and "Help" buttons are at the bottom.
- Properties Panel:** Located at the bottom left, it has a "Filter: All" dropdown and a table with columns "Property Name" and "Value".
- Jobs Panel:** Located at the bottom right, it has a table with columns "Description", "Job Id", "Gateway", and "Server".
- Taskbar:** Shows the Windows taskbar with various application icons and the system clock at 11:20.

The screenshot shows the Materials Studio interface with the following components:

- Project Panel:** Shows a tree view for 'BiInO3' with a sub-folder '3D Atomistic CASTEP GeomOpt' containing files like '3D Atomistic - Calculation', '3D Atomistic.xsd', 'Status.txt', '3D Atomistic Energies.xcd', '3D Atomistic Convergence.xcd', '3D Atomistic.xtd', '3D Atomistic.param', '3D Atomistic.castep', and '3D Atomistic.xsd'.
- CASTEP Calculation Dialog:** Has tabs for 'Setup', 'Electronic', 'Properties', and 'Job Control'. Under 'Setup', 'Density of states' is checked. Other options include 'Electron density difference', 'Electron localization function', 'NMR', 'Optical properties', and 'Orbitals'. 'Density of states' parameters are set to 'Empty bands: 20' and 'k-point set: Ultra_fine 6x6x6'. 'Calculate PDOS' is checked. A 'More...' button is highlighted with a yellow callout.
- CASTEP Density of States Options Dialog:** Shows 'DOS k-points' with 'Quality' set to 'Ultra-fine' and 'Separation' to '0,04 1/Å'. 'Monkhorst-Pack grid' parameters are 'a: 6, b: 6, c: 6'. 'Actual spacing' is '0,039759 0,039759 0,039759 1/Å'. 'Origin shift' is '0,0 0,0 0,0'. 'Functional' is 'GGA PBE' and 'Band energy tolerance' is '1,0e-5 eV'.
- Properties Panel:** Shows a table with columns 'Property' and 'Value'.

Property	Value
Name	
Style	
- Job Queue Table:** Has columns 'Description', 'Job Id', 'Gateway', 'Server', and 'Status'.

Callout Text: Vous pouvez optimiser les paramètres pour Le calcul du TDOS et PDOS

BiInO3 - Materials Studio - [3D Atomistic CASTEP GeomOpt\3D Atomistic.xsd]

File Edit View Modify Build Tools Statistics Modules Window Help

Project

BiInO3

- 3D Atomistic CASTEP GeomOpt
 - 3D Atomistic - Calculation
 - 3D Atomistic.xsd
 - Status.txt
 - 3D Atomistic Energies.xcd
 - 3D Atomistic Convergence.xcd
 - 3D Atomistic.xtd
 - 3D Atomistic.param
 - 3D Atomistic.castep
 - 3D Atomistic.xsd

CASTEP Calculation

Setup | Electronic | Properties | Job Control

- Electron density difference
- Electron localization function
- NMR
- Optical properties
- Orbitals
- Phonons

Electron density difference

- Atomic densities
- Sets of atoms
- Both atomic densities and sets of atoms

Run Files... Help

Properties

Filter: All

Property	Value
Name	
Style	

Jobs

Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...

Ready

FR 11:24

The screenshot displays the Materials Studio interface for a BiInO3 project. The 'CASTEP Calculation' dialog box is open, with the 'Optical properties' checkbox selected. The 'k-point set' is set to 'Customized' with a '20x20x20' grid. A yellow callout bubble points to the 'More...' button in the 'CASTEP Calculation' dialog, indicating that users can optimize parameters for optical property calculations.

The 'CASTEP Optical Properties Options' dialog box is also open, showing the following settings:

- Optics k-points:
 - Gamma point only
 - Quality: Ultra-fine
 - Separation: 0.05 1/Å
 - Custom grid parameters
- Monkhorst-Pack grid:
 - Grid parameters: a=20, b=20, c=20
 - Actual spacing: 0.011928, 0.011928, 0.011928 1/Å
 - Origin shift: 0.0, 0.0, 0.0
- Use separate XC functional for optics calculation
- Functional: GGA, PBE
- Band energy tolerance: 1.0e-5 eV

Vous pouvez optimiser les paramètres pour Le calcul du propriétés optique

BiInO3 - Materials Studio - [3D Atomistic CASTEP GeomOpt\3D Atomistic.xsd]

File Edit View Modify Build Tools Statistics Modules Window Help

Project

- BiInO3
 - 3D Atomistic CASTEP GeomOpt
 - 3D Atomistic - Calculation
 - 3D Atomistic.xsd
 - Status.txt
 - 3D Atomistic Energies.xcd
 - 3D Atomistic Convergence.xcd
 - 3D Atomistic.xtd
 - 3D Atomistic.param
 - 3D Atomistic.castep
 - 3D Atomistic.xsd

CASTEP Calculation

Setup | Electronic | Properties | Job Control

- Optical properties
- Orbitals
- Phonons
- Polarizability and IR spectrum
- Population analysis
- Stress

Population analysis

Distance cut-off for bond populations: 5.0 Å

- Calculate band populations

Run Files... Help

Properties

Filter: All

Property	Value
Name	
Style	

Jobs

Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...
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Ready

FR 11:40

Introduire le chiffre qui est relatif aux paramètres du réseau cristallin

Analyse des résultats
Pour les propriétés électroniques
et optiques

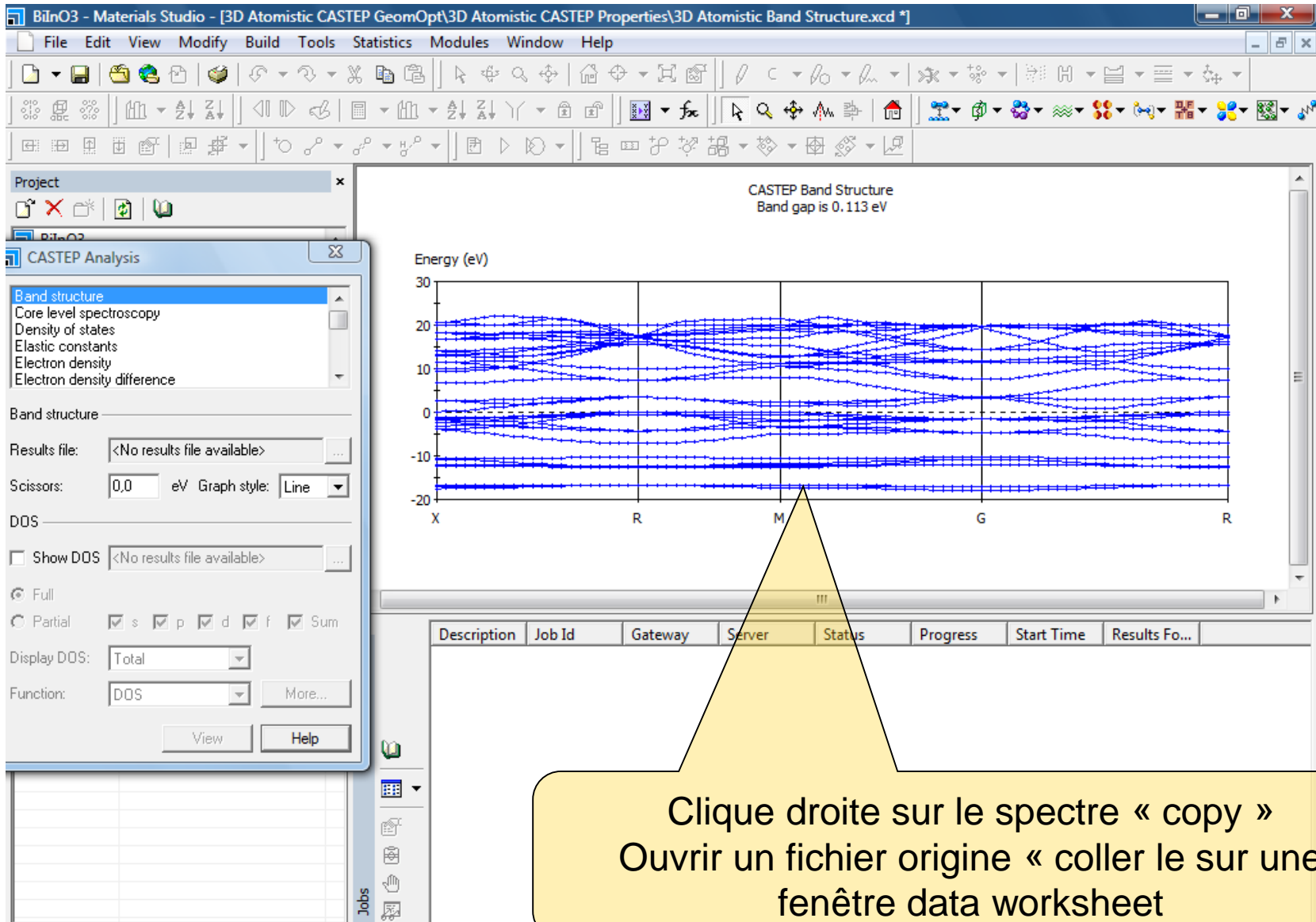
Analyse des Propriétés électronique

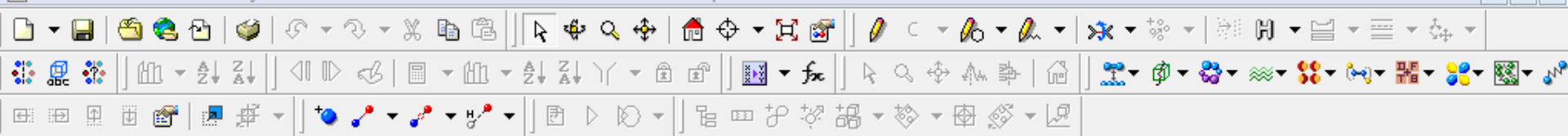
The screenshot shows the Materials Studio interface with the CASTEP Analysis dialog box open. The dialog box has the following settings:

- Band structure: Selected
- Results file: 3D Atomistic CASTEP Properties\...
- Scissors: 0,0 eV Graph style: Line
- DOS: Show DOS 3D Atomistic CASTEP Properties\...
- Full: Partial: s: p: d: f: Sum:
- Display DOS: Total
- Function: DOS

The 3D model shows a crystal structure with Bi atoms (purple spheres) and O atoms (red spheres). The CASTEP Analysis dialog box is overlaid on the model, and a yellow callout bubble points to the 'View' button.

Cliquer sur « view » pour visualiser
Le spectre énergétique du « band structure »





Project

- 3D Atomistic - Calculation
 - Status.txt
 - 3D Atomistic_PopAnl-DensDiff,
 - 3D Atomistic_PopAnl-DensDiff,
 - 3D Atomistic_BandStr.param
 - 3D Atomistic_BandStr.castep
 - 3D Atomistic_DOS.param
 - 3D Atomistic_DOS.castep
 - 3D Atomistic_Optics.param
 - 3D Atomistic_Optics.castep
 - 3D Atomistic Band Structure.xc
- 3D Atomistic - Calculation
 - 3D Atomistic.xsd
 - Status.txt
 - 3D Atomistic Energies.xcd

CASTEP Analysis

- Band structure
- Core level spectroscopy
- Density of states
- Elastic constants
- Electron density
- Electron density difference

Density of states

Results file: 3D Atomistic CASTEP Properties\...

Full
 Partial

Display DOS: Total

Function: DOS

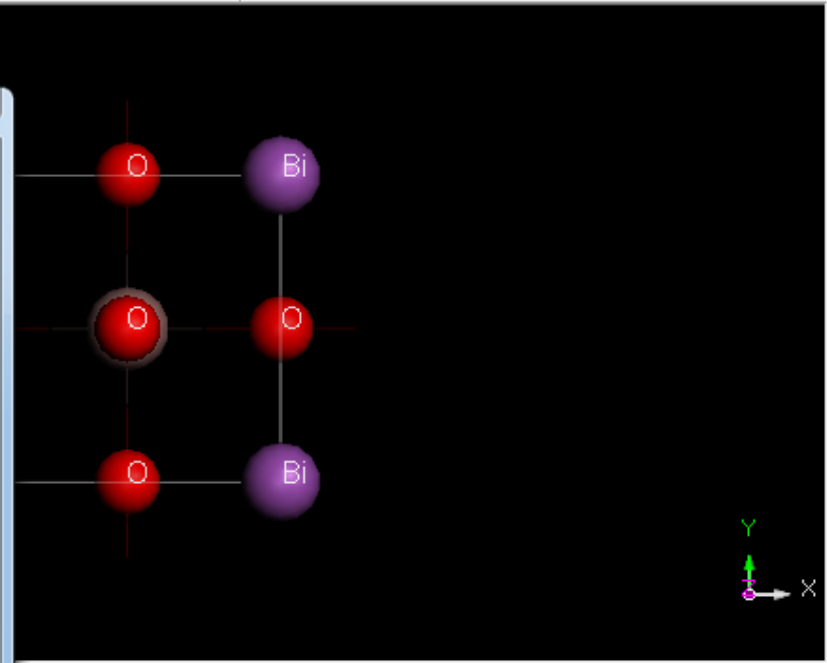
Scissors: 0,0 eV

Atom Selection

More...

View

Help



CASTEP DOS Analysis Options

Integration method: Interpolation

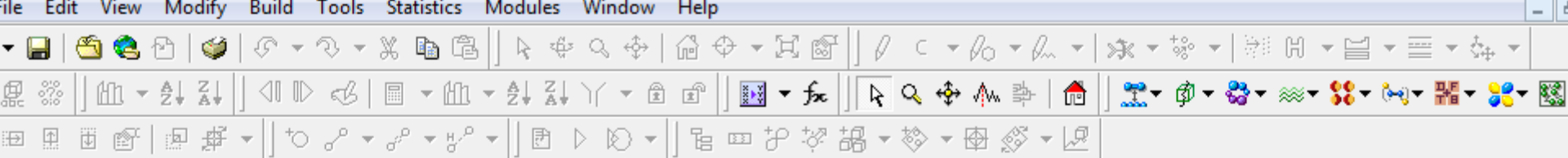
Smearing width: 0,2 eV

Accuracy level: Coarse

Instrument broadening: 0,05 eV

OK Cancel Help

Cliquer sur « view » pour visualiser le spectre TDOS



Project

- 3D Atomistic - Calculation
- Status.txt
- 3D Atomistic_PopAnl-DensDiff
- 3D Atomistic_PopAnl-DensDiff

CASTEP Analysis

Band structure
Core level spectroscopy
Density of states
Elastic constants
Electron density
Electron density difference

Density of states

Results file: <No results file available>

Full
Partial s p d f Sum

Display DOS: Total

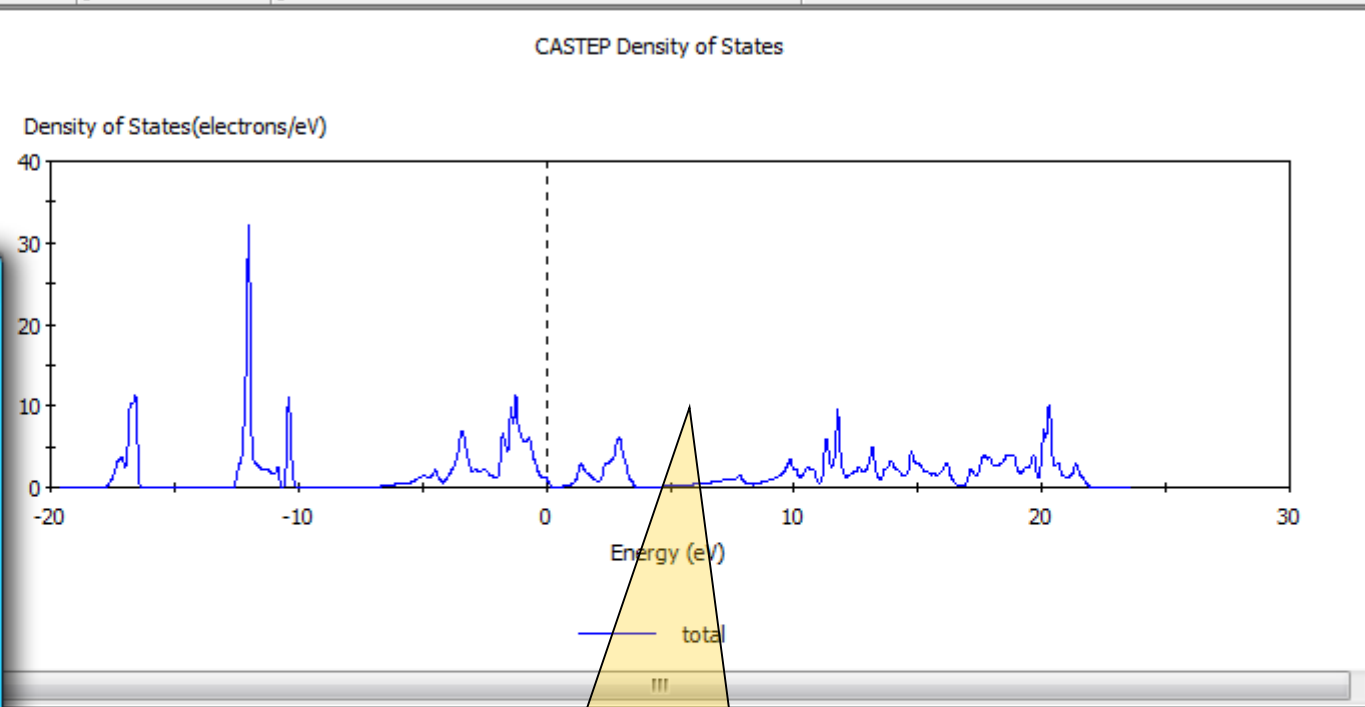
Function: DOS

Scissors: 0.0 eV

Atom Selection

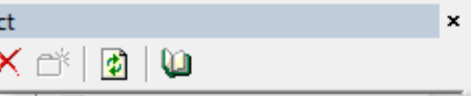
More...

View Help



Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...

Clique droite sur le spectre « copy »
Ouvrir un fichier origine « coller le sur un
fenêtre data worksheet



CASTEP Analysis

- Band structure
- Core level spectroscopy
- Density of states**
- Elastic constants
- Electron density
- Electron density difference

Density of states

Results file: 3D Atomistic CASTEP Properties\3 ...

Full

Partial s p d f Sum

Display DOS: Total

Function: DOS

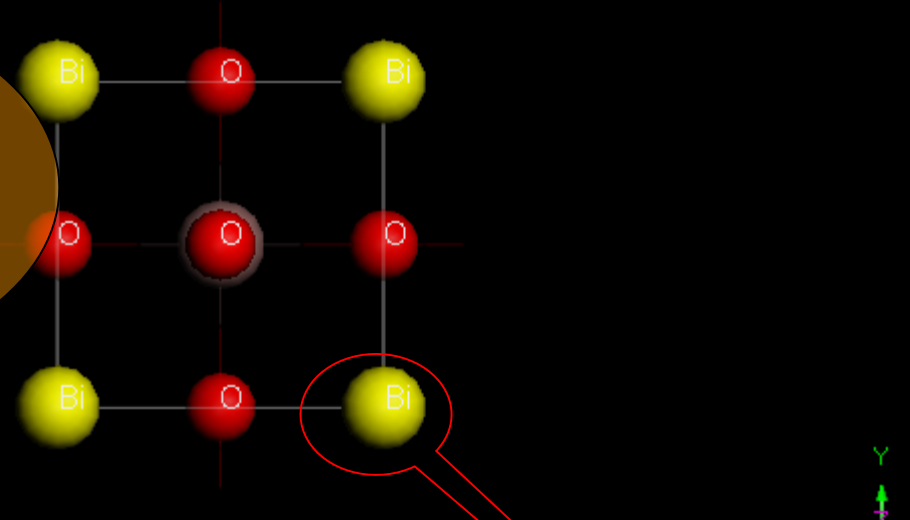
Scissors: 0,0 eV

Atom Selection

More...

View Help

Cliquer sur « view » pour obtenir le spectre PDOS « Bi »



Atom Selection

Select by Property: Select All Deselect All

Element

Is Bi

Selection mode

- Create a new selection from all visible atoms
- Select from the existing selection
- Add to the existing selection

Select Help

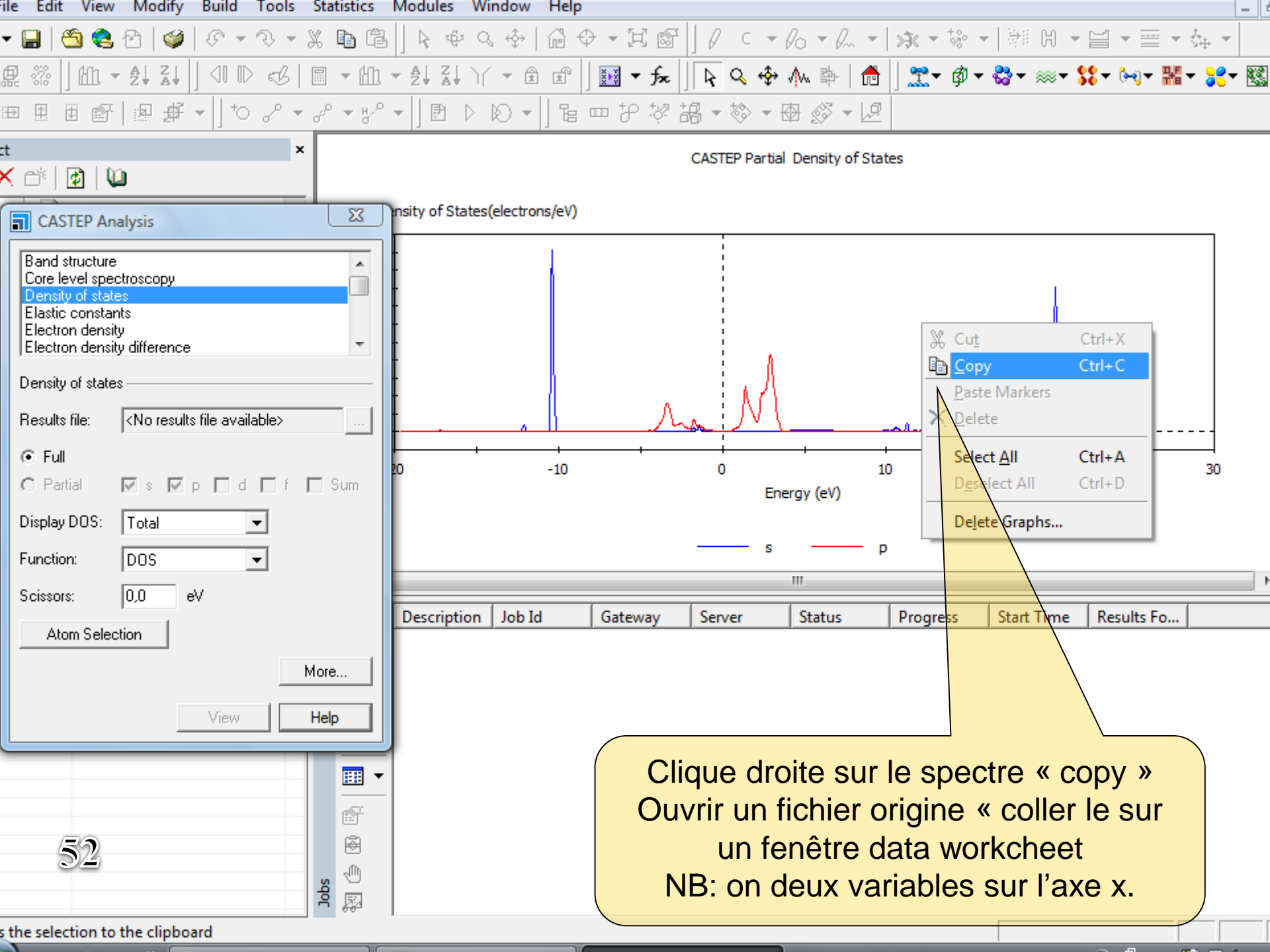
Periodic Table

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
H														
Li	Be											B	C	N
Na	Mg											Al	Si	P
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb
Cs	Ba	Lu	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi
Fr	Ra	Lr	Rf	Db	Sg	Bh	Hs	Mt	Uun	Uuu	Uub	Uut	Uuq	Uup
La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm		
Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md		

Element: Bismuth Atomic No. 83

51

Jobs



CASTEP Partial Density of States

Density of States(electrons/eV)

CASTEP Analysis

- Band structure
- Core level spectroscopy
- Density of states**
- Elastic constants
- Electron density
- Electron density difference

Density of states

Results file: <No results file available>

Full
 Partial

s p d f Sum

Display DOS: Total

Function: DOS

Scissors: 0,0 eV

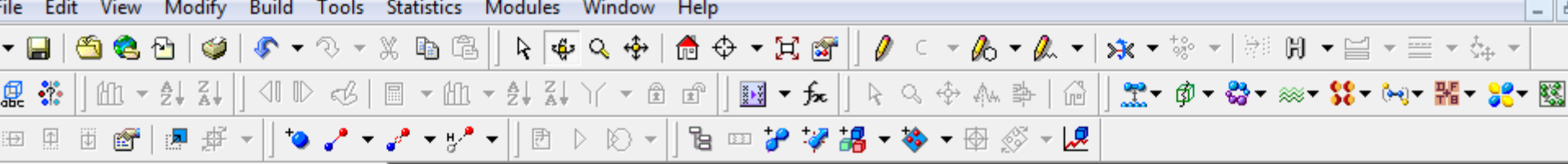
Atom Selection

More...

View Help

- Cut Ctrl+X
- Copy Ctrl+C**
- Paste Markers
- Delete
- Select All Ctrl+A
- Deselect All Ctrl+D
- Delete Graphs...

Clique droite sur le spectre « copy »
Ouvrir un fichier origine « coller le sur
un fenetre data workcheet
NB: on deux variables sur l'axe x.



CASTEP Analysis

- IR spectrum
- NMR
- Optical properties**
- Orbitals
- Phonon dispersion
- Phonon density of states

Optical properties

Results file: 3D Atomistic CASTEP Properties\...

Calculation: Polycrystalline

Smearing: 0,5 eV Scissors: 0,0 eV

Polarization: 1,0 0,0 0,0

View properties

Function: Absorption

Units: eV

More...

Calculate View Help

	A	B	C	D
(eV)	Calculation	Direction	Smearing (eV)	
000	Polycrystalline	N/A	0,50000000	

Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...
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Appuyer sur « calculate »
puis sur « view » pour
visualiser le spectre de la
grandeur optique voulue, par
exemple
« Adsorption »

Calcul des constantes élastiques

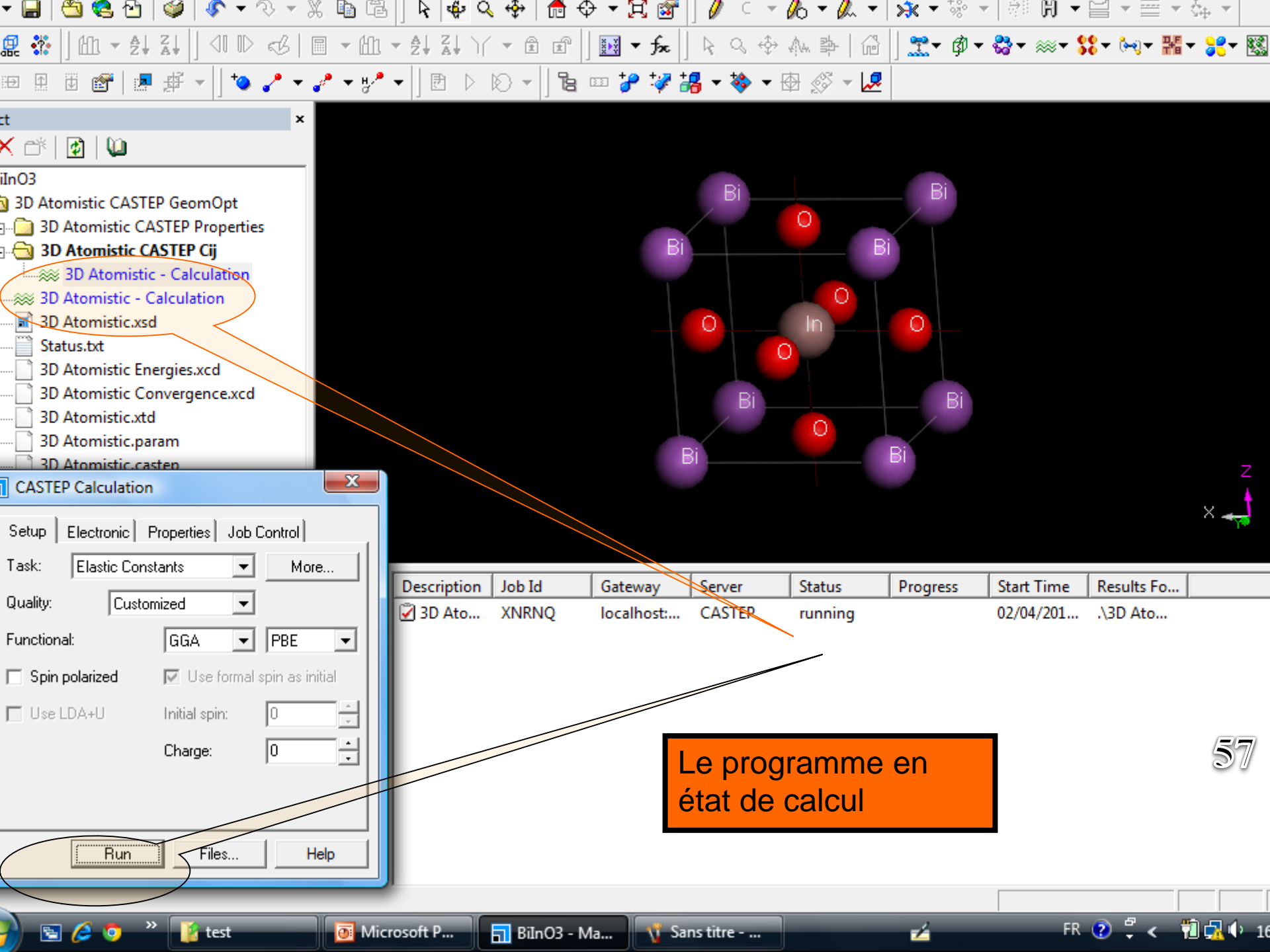
« Propriétés élastique »

The screenshot displays the Materials Studio interface for a BiInO3 project. The 'CASTEP' menu is open, showing 'Calculation' and 'Analysis' options. The 'CASTEP Calculation' dialog box is active, with the 'Task' set to 'Elastic Constants'. The 'Quality' is set to 'Customized', and the 'Functional' is set to 'GGA' and 'PBE'. The 'CASTEP Elastic Constants' dialog box is also open, showing the 'Number of steps for each strain' set to 6 and the 'Maximum strain amplitude' set to 0.003. The 'Strain pattern' table is visible, showing a single strain component.

#	xx	yy	zz	yz	zx	xy
1	1	0	0	1	0	0

3D Atomisticdocument.xsd optimisé

Opens the CASTEP Calculation tool



Le programme en état de calcul

Analyse des constants élastiques

Job Completed

Job: [XNRNQ] - 3D Atomistic CASTEP Cij
Program: CASTEP
Gateway: My Computer
Status: successfully-completed

OK

Host: PC-de-mounir
16:58:37 2013

```
CCC  AA  SSS  TTTT  EEEEE  PPPP  
C   A  A  S   T   E   P  P  
C   AAAA SS   T   EEE  PPPP  
C   A  A  S   T   E   P  
CCC  A  A  SSS  T   EEEEE  P
```

welcome to Materials Studio CASTEP version 4.4
Ab Initio Total Energy Program

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Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...

Properties

Filter:

Property	Value

Jobs

Fin de calcul
Des C_{ij}