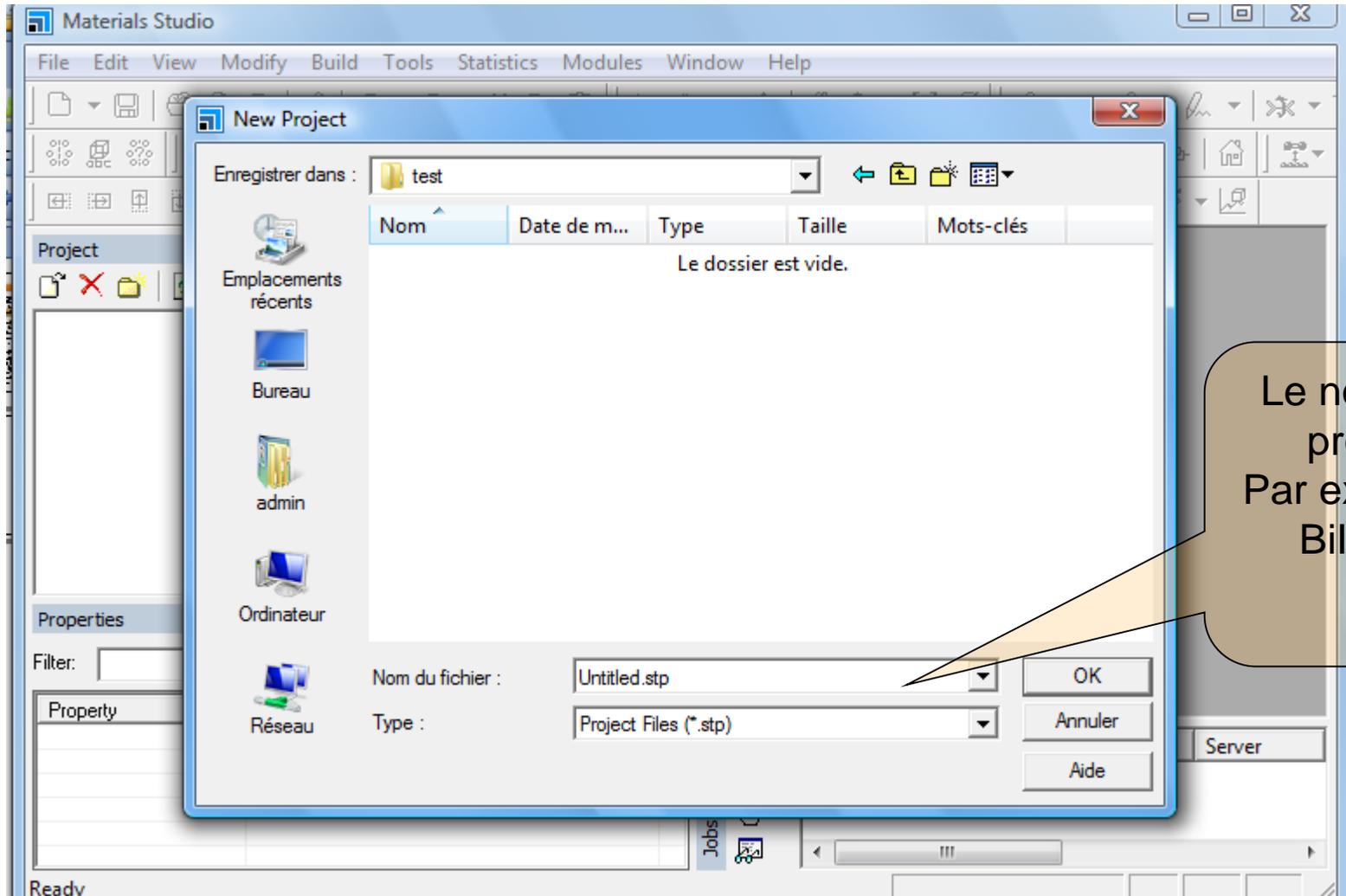


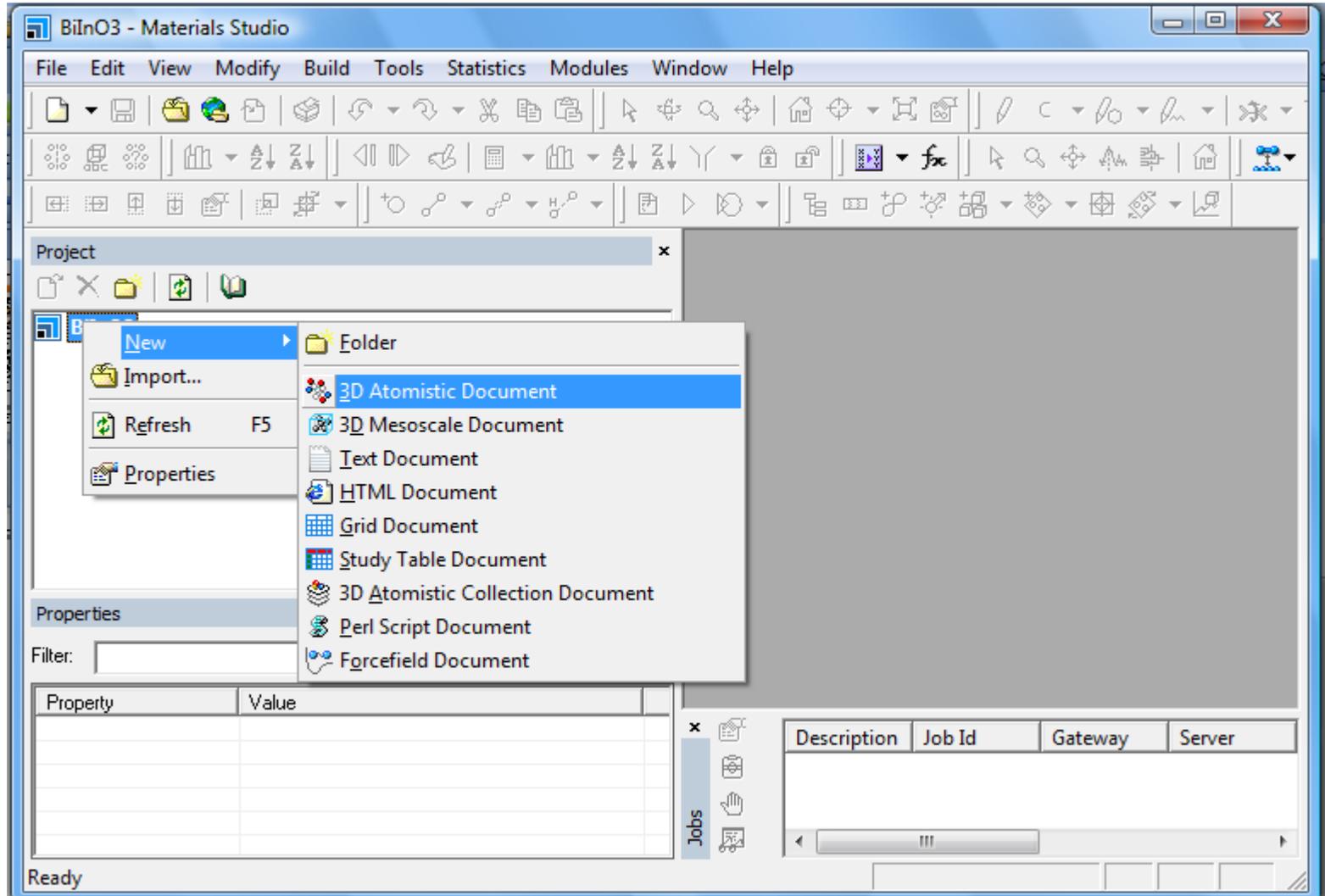
بِسْمِ اللَّهِ الرَّحْمَنِ الرَّحِيمِ

انشاء برنامج الحساب
CASTEP

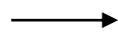
Cambridge Sequential Total Energy Package

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

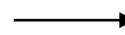




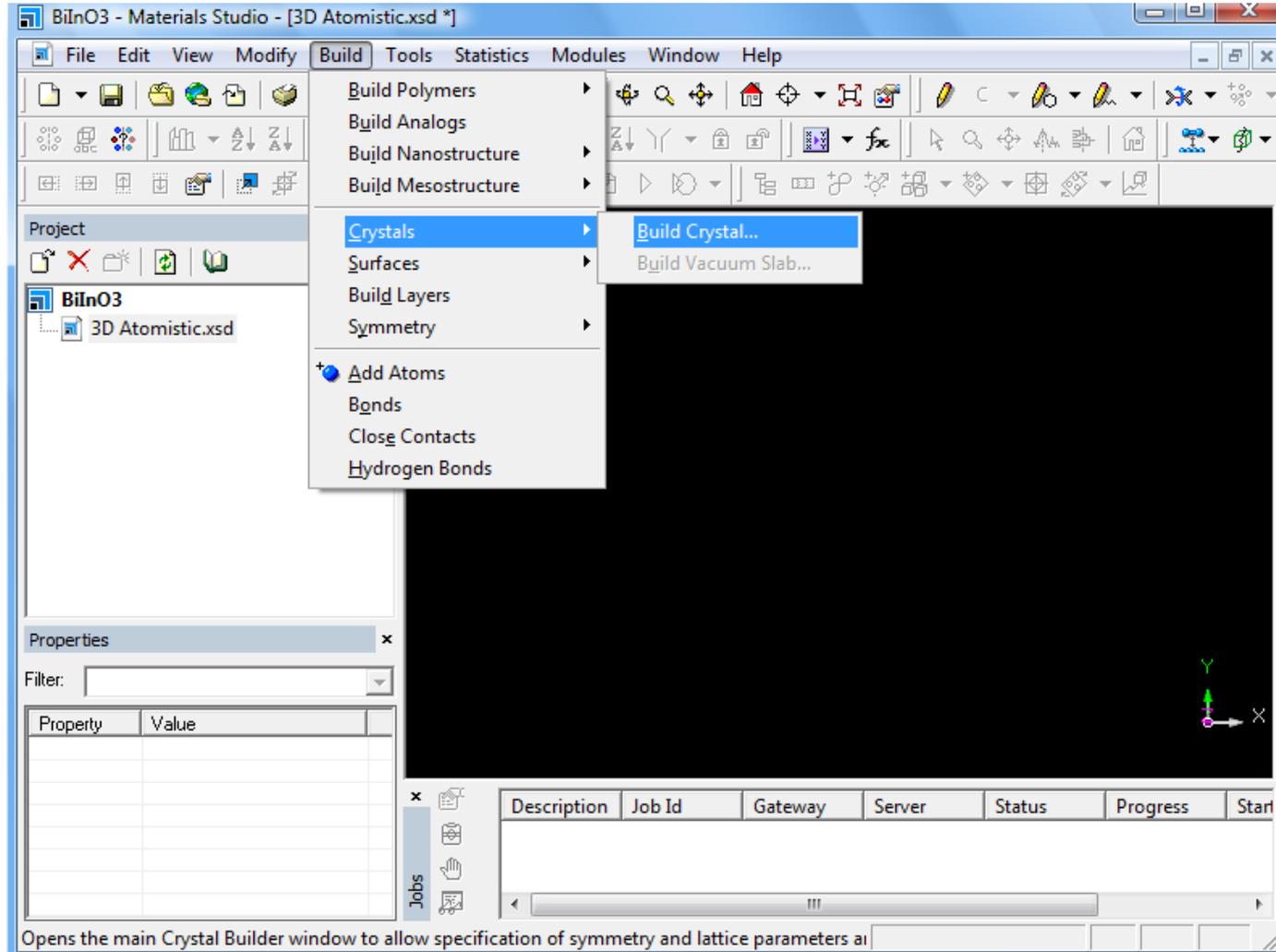
Appuyer sur Build



Crystals



Build
crystal



Build
Crystal

Space
group

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

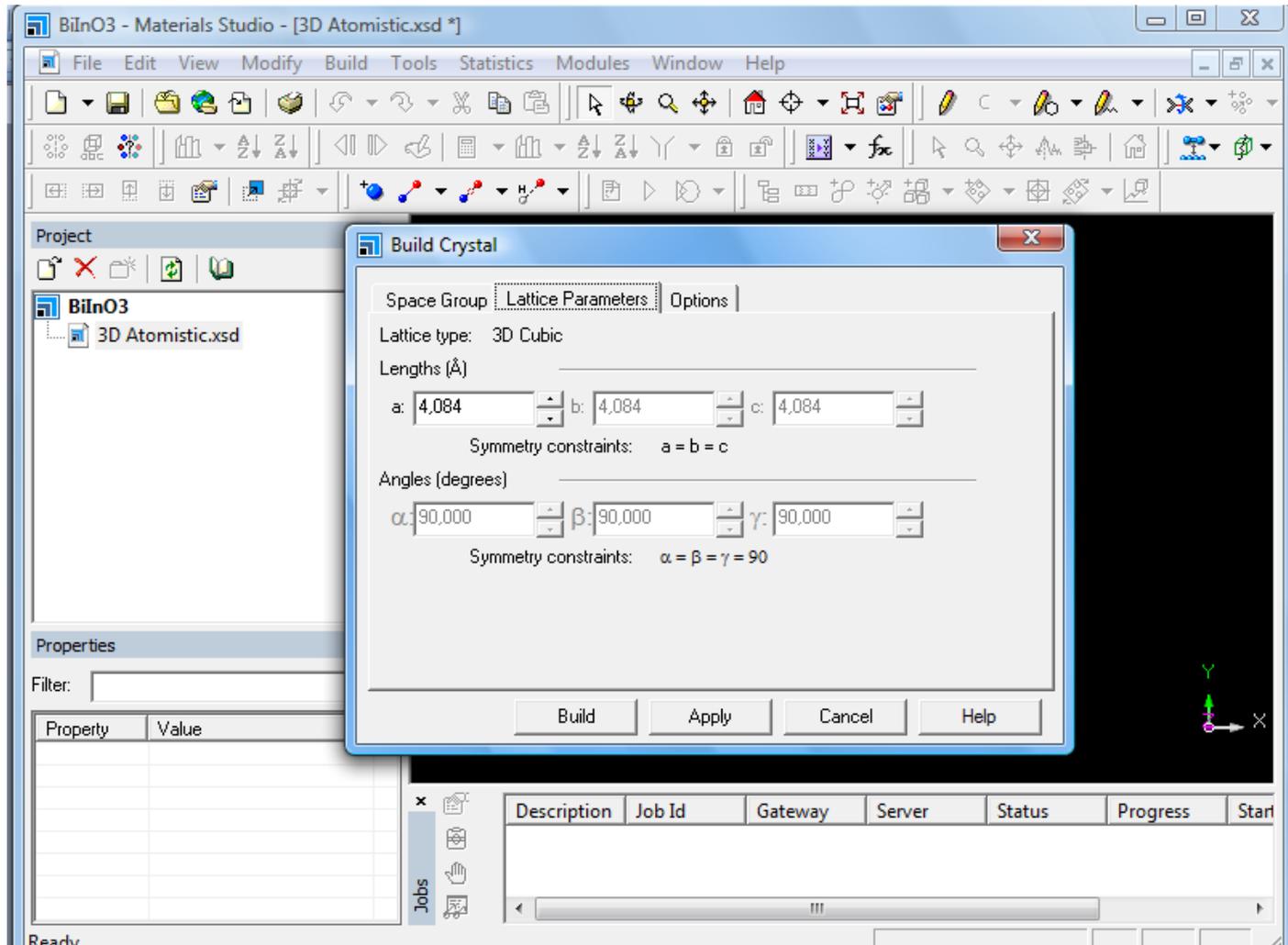
The screenshot shows the Materials Studio interface with the 'Build Crystal' dialog box open. The dialog has three tabs: 'Space Group', 'Lattice Parameters', and 'Options'. The 'Space Group' tab is active, showing a list of space groups. The 'Enter group' field is set to '221 PM-3M'. The 'List' dropdown 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

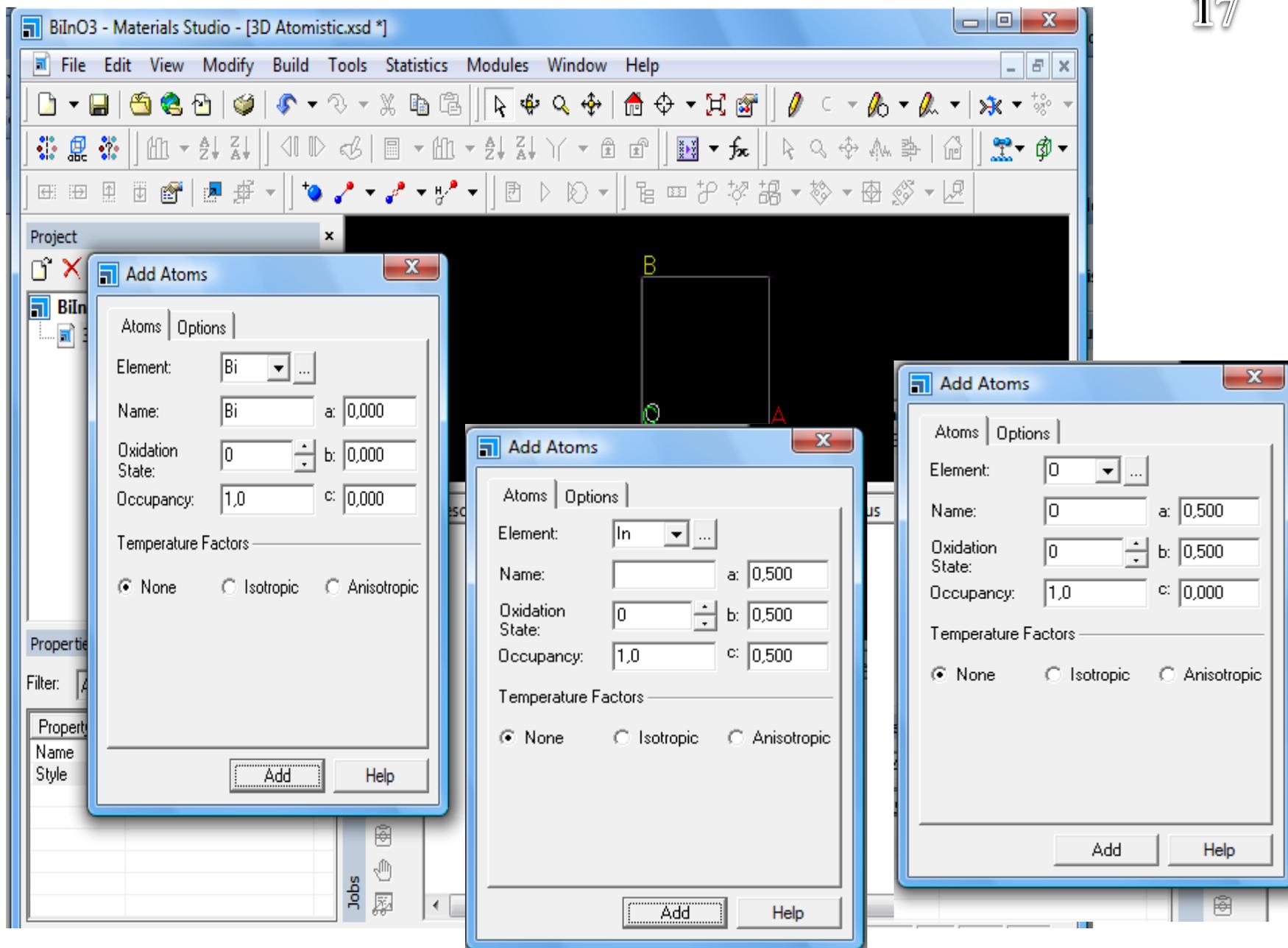
The screenshot shows the Materials Studio interface with the 'Build' menu open. The 'Add Atoms' option is highlighted in blue. The main 3D view is currently empty, with a coordinate system (X, Y, Z) visible in the bottom right corner. The 'Project' panel on the left shows the current project 'BiInO3' 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



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.

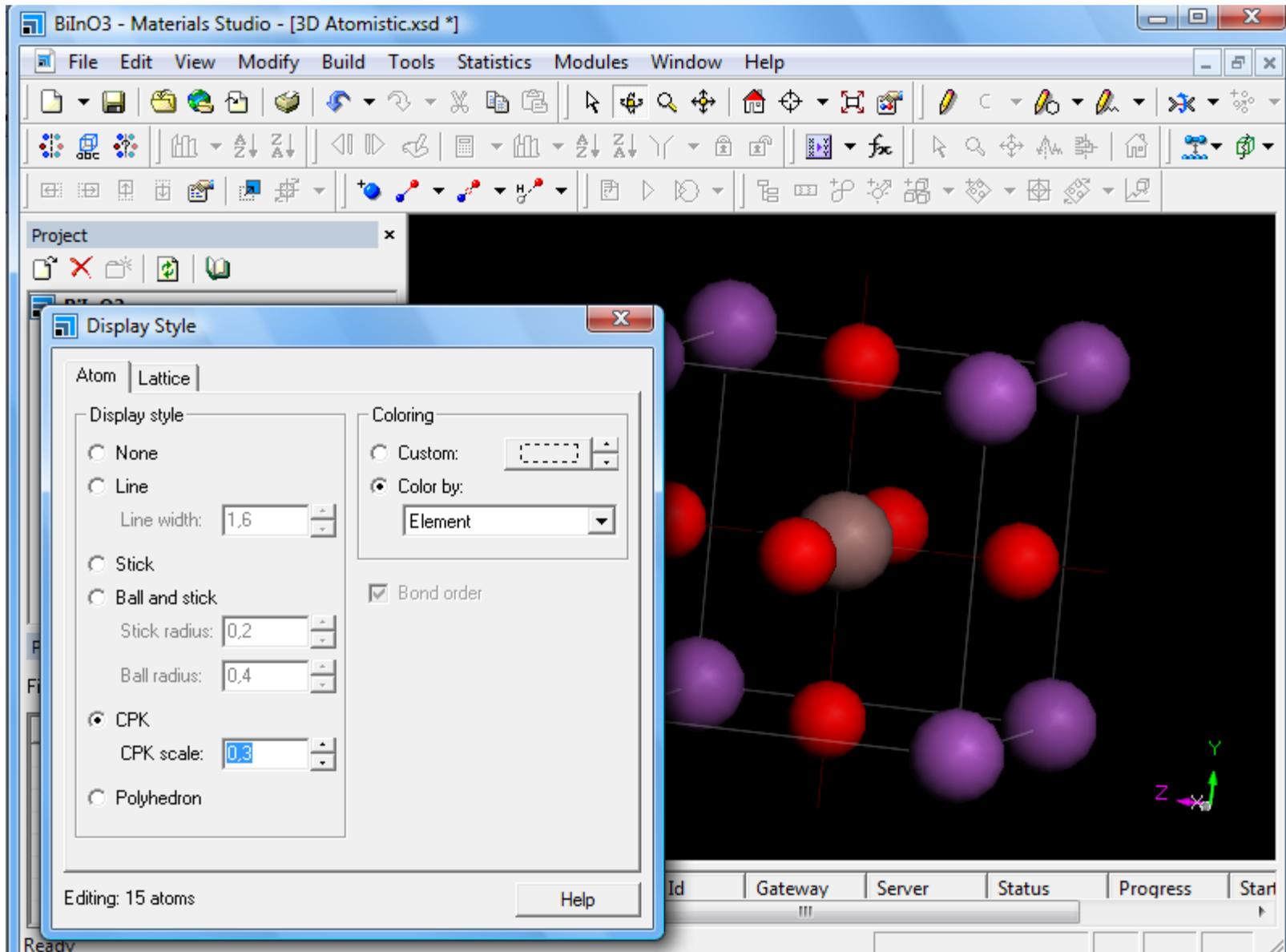
Property	Value
Charge	0,000000
Composition	
ElementNa...	
ElementSy...	
ForcefieldT...	
FormalChar...	
FormalSpin	0
FormalSpin...	Undefined

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 displays the Materials Studio interface for a 3D atomic model of BiInO3. A context menu is open over the model, with the 'Label' option highlighted. The interface includes a menu bar (File, Edit, View, Modify, Build, Tools, Statistics, Modules, Window, Help), a toolbar, a Project panel, a Properties panel, and a Job panel.

Project Panel:

- BiInO3
 - 3D Atomistic.xsd

Properties Panel:

Filter: Atom

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

Job Panel:

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 3D model shows Bi atoms (purple), In atoms (grey), and O atoms (red) connected by bonds. A coordinate system (x, y, z) is visible in the bottom right corner of the 3D view.

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

Description	Job Id	Gateway	Server	Status	Progress	Start

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 at the bottom.

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 CASTEP Calculation tool

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

- CASTEP Calculation:**
 - Task: Geometry Optimization
 - Quality: Ultra-fine
 - Functional: GGA, PBE
 - Spin polarized:
 - Use formal spin as initial:
 - Use LDA+U:
 - Initial spin: 0
 - Charge: 0
- CASTEP Geometry Optimization:**
 - Minimizer: Selected
 - Options: Options
 - Stress: Stress
 - Convergence tolerance:
 - Quality: Ultra-fine
 - Energy: 5.0e-6 eV/atom
 - Max. force: 0.01 eV/Å
 - Max. stress: 0.02 GPa
 - Max. displacement: 5.0e-4 Å
 - Max. iterations: 100
 - Optimize cell:
 - Cell optimization: Fixed Basis Quality
 - Compressibility: Hard

Arrows indicate the flow from the 'More...' button in the CASTEP Calculation dialog to the 'Minimizer' tab in the CASTEP Geometry Optimization dialog.

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 'Setup' tab with '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). Other fields include 'Initial spin' (0) and 'Charge' (0).
- CASTEP Geometry Optimization:** Shows the 'Minimizer' tab with 'Algorithm' set to 'BFGS'. There are checkboxes for 'Use delocalized internals' (unchecked) and 'Auto-update time step' (unchecked). Other settings include 'Damping algorithm' (Independent), 'Damping coefficient recalculation frequency' (30), and 'Wavefunction extrapolation' (1st W).

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'. 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

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 with two dialog boxes open. The 'CASTEP Electronic Options' dialog is on the left, and the 'CASTEP Calculation' dialog is on the right. An arrow points from the 'Use custom energy cut-off' field in the Electronic Options dialog to the 'Energy cutoff' field in the Calculation dialog.

CASTEP Electronic Options

- Basis: SCF | k-points | Potentials
- Use custom energy cut-off: 380,0 eV
- FFT grid: _____
- Derived grid: Precise
- Divisions: a*: 30, b*: 30, c*: 30
- Finite basis correction: _____
- Apply finite basis set correction: Smart
- Correction mode: Automatic
- Numerical differentiation using 3 points
- Energy derivative w.r.t. cutoff: 0,0 eV

CASTEP Calculation

- Setup | Electronic | Properties | Job Control
- Energy cutoff: Customized 380,0eV
- SCF tolerance: Ultra-fine
- k-point set: Fine 6x6x6
- Pseudopotentials: Ultrasoft
- Pseudopotential representation: Reciprocal space
- Use core hole
- More...
- Run | Files... | Help

At the bottom of the window, a table header is visible:

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

More...

Run Files... Help

Property Charge Compos Element Element Forcefield FormalChar... FormalSpin 0 FormalSpin... Undefined

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 'My Computer', and 'Run in parallel on' is set to 2 of 2 processors. The 'Run' button is highlighted by 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.

Project: BiInO3
3D Atomistic.xsd

Properties: Filter: Atom

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

Job x

Description	Job Id	Gateway	Server	Status	Progress	Start

Ready

BiInO3 - 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	

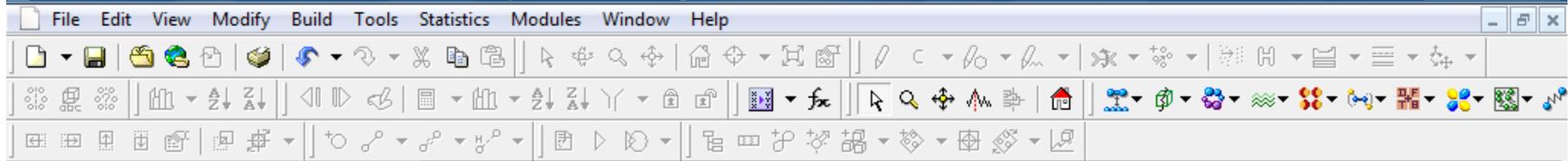
Jobs

Description	Job Id	Gateway	Server	Status	Progress	Start Time	Results Fo...
<input checked="" type="checkbox"/> 3D Ato...	X6RUL	localhost...	CASTEP	running		02/04/201...	.\3D Ato...

Ready

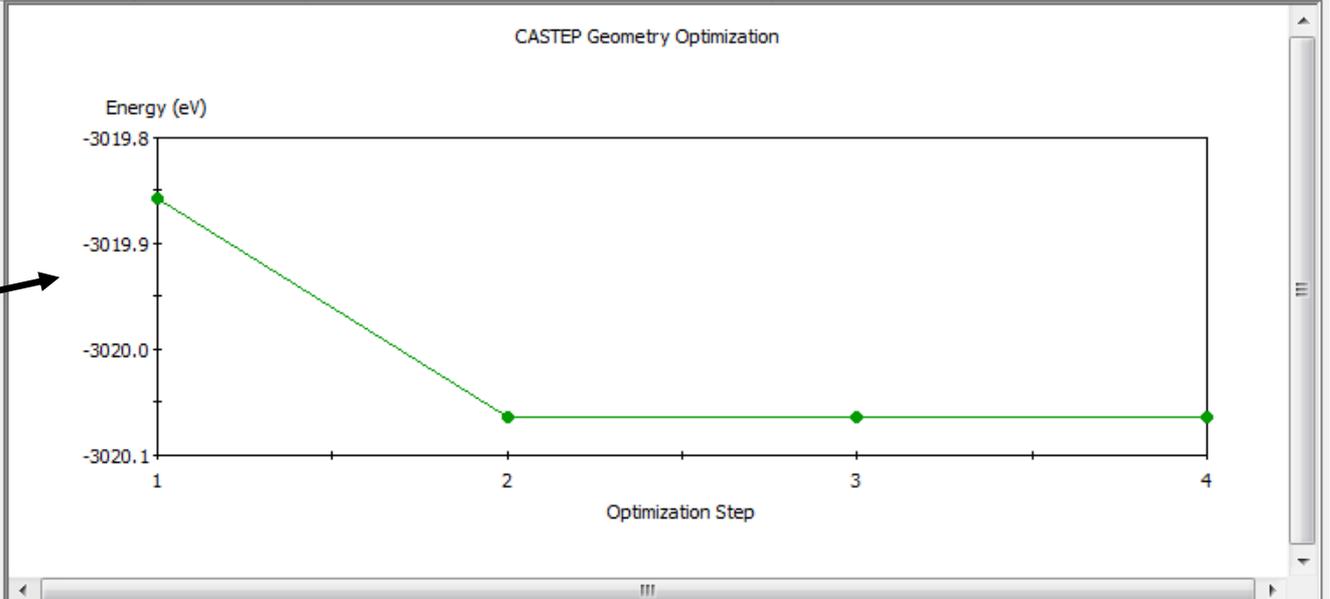
FR 10:56

Le programme en état de calcul



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 at the bottom left is empty, and the 'Jobs' window at the bottom right shows a table with columns for Description, Job Id, Gateway, Server, Status, Progress, Start Time, and Results Fo....

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, with a filter set to "All" and a table with columns "Property Name" and "Style".
- Jobs Panel:** Located at the bottom right, with columns "Description", "Job Id", "Gateway", and "Server".
- Taskbar:** Shows the Windows taskbar with various application icons and a system tray with the time "11:20".

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

- Density of states
- Electron density difference
- Electron localization function
- NMR
- Optical properties
- Orbitals

Density of states:

Empty bands: 20

k-point set: Ultra_fine 6x6x6

Calculate PDOS

More...

Run Files... Help

CASTEP Density of States Options

DOS k-points:

- Gamma point only
- Quality: Ultra-fine
- Separation: 0,04 1/Å
- Custom grid parameters

Monkhorst-Pack grid

Grid parameters: a: 6, b: 6, c: 6

Actual spacing: 0,039759, 0,039759, 0,039759 1/Å

Origin shift: 0,0, 0,0, 0,0

Display points...

Use separate XC functional for DOS calculation

Functional: GGA, PBE

Band energy tolerance: 1,0e-5 eV

Help

Properties

Filter: All

Property	Value
Name	
Style	

Description Job Id Gateway Server Status

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

Ready

FR 11:22

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

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

Optical properties

Empty bands: 20

k-point set: Customized 20x20x20

More...

Run Files... Help

CASTEP Optical Properties Options

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

Display points...

- Use separate XC functional for optics calculation

Functional: GGA PBE

Band energy tolerance: 1.0e-5 eV

Help

Properties

Filter: All

Property	Value
Name	
Style	

Ready

FR 11:36

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

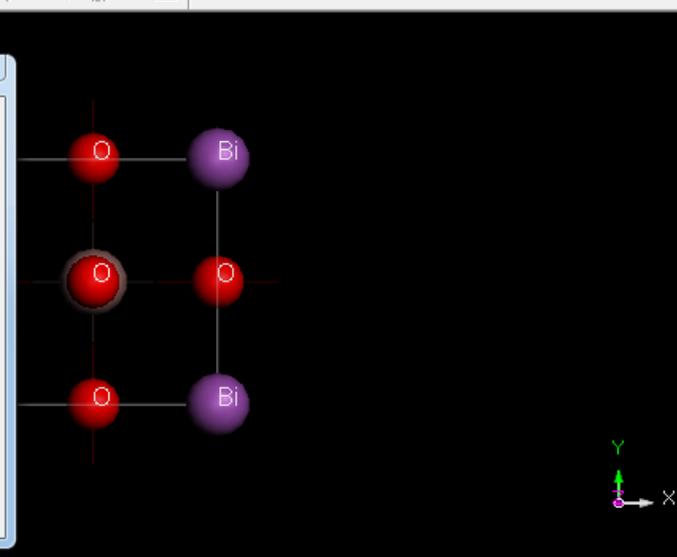
Property	Value
Name	
Style	

Jobs

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

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 for a BiInO3 project. The CASTEP Analysis dialog box is open, with 'Band structure' selected in the list. The 'View' button is highlighted by a yellow callout bubble.

CASTEP Analysis

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

Band structure

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

Scissors: 0,0 eV Graph style: Line

DOS

Show DOS 3D Atomistic CASTEP Properties\...

Full

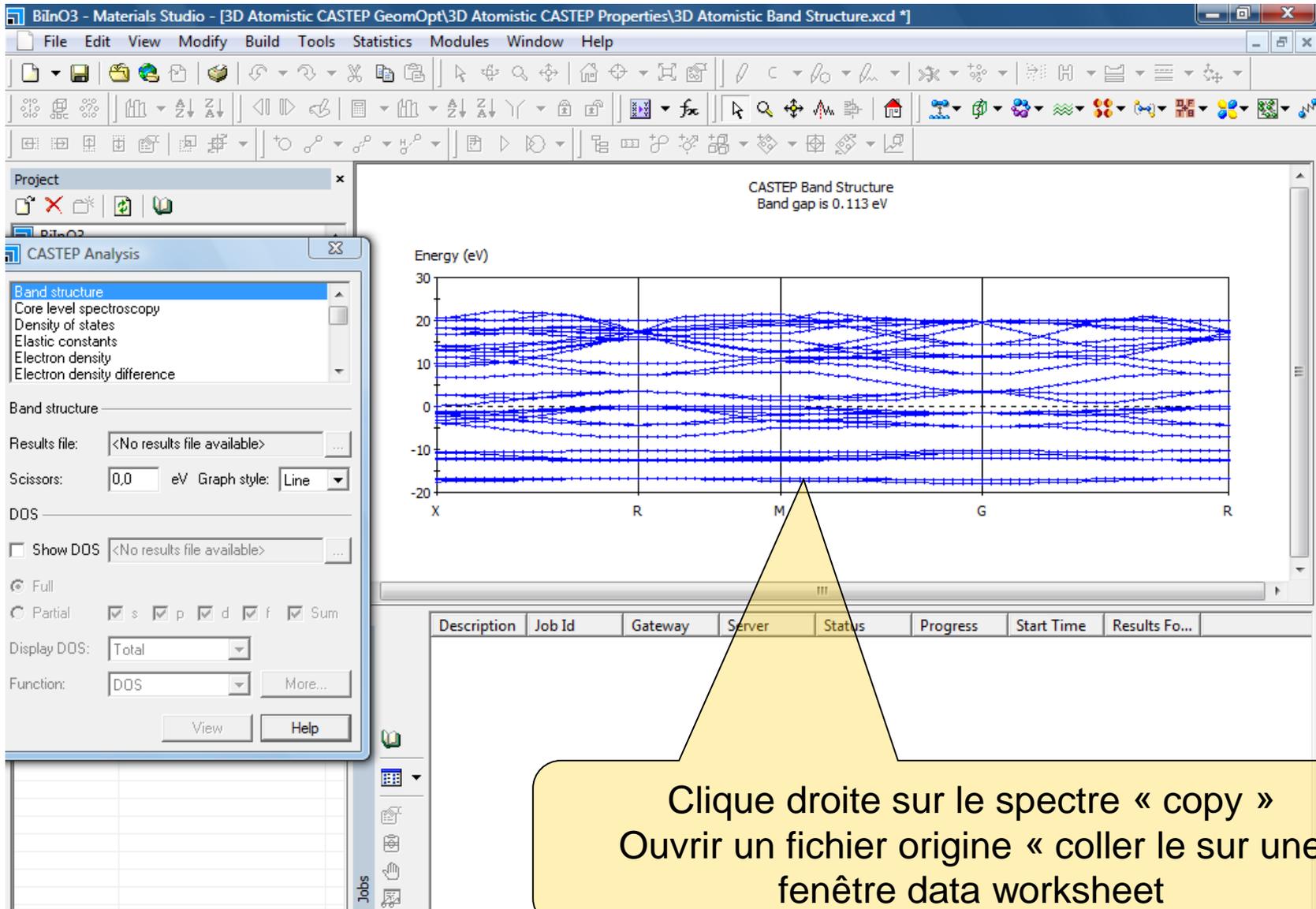
Partial s p d f Sum

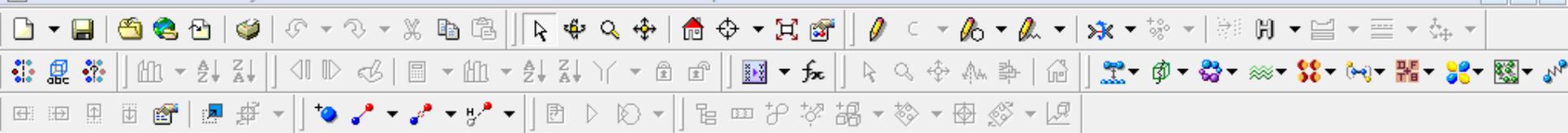
Display DOS: Total

Function: DOS More...

View Help

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

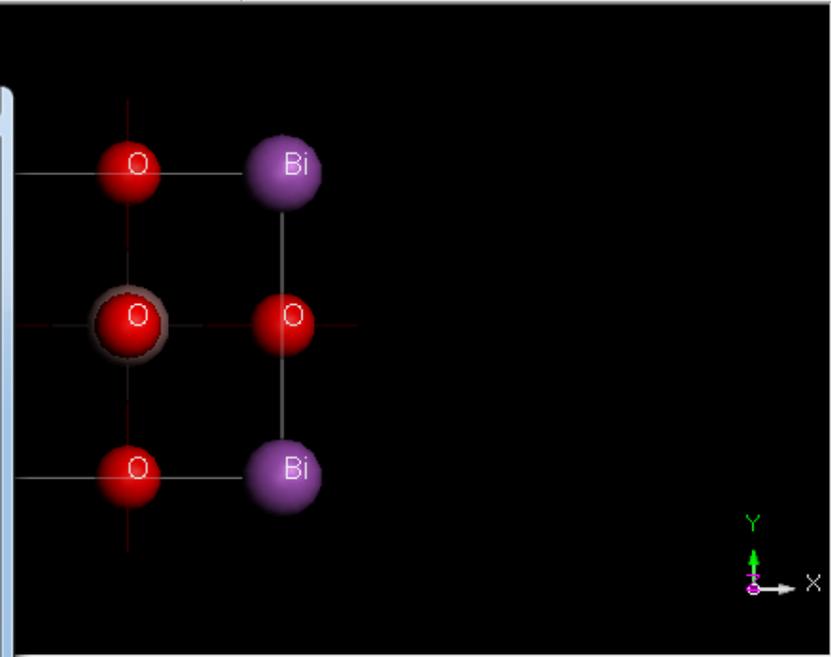
Function: DOS

Scissors: 0,0 eV

Atom Selection

More...

View Help



CASTEP DOS Analysis Options

Integration method: Interpolation

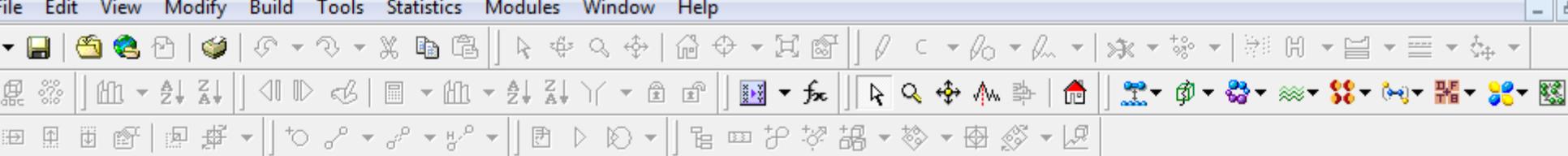
Smearing width: 0,2 eV

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

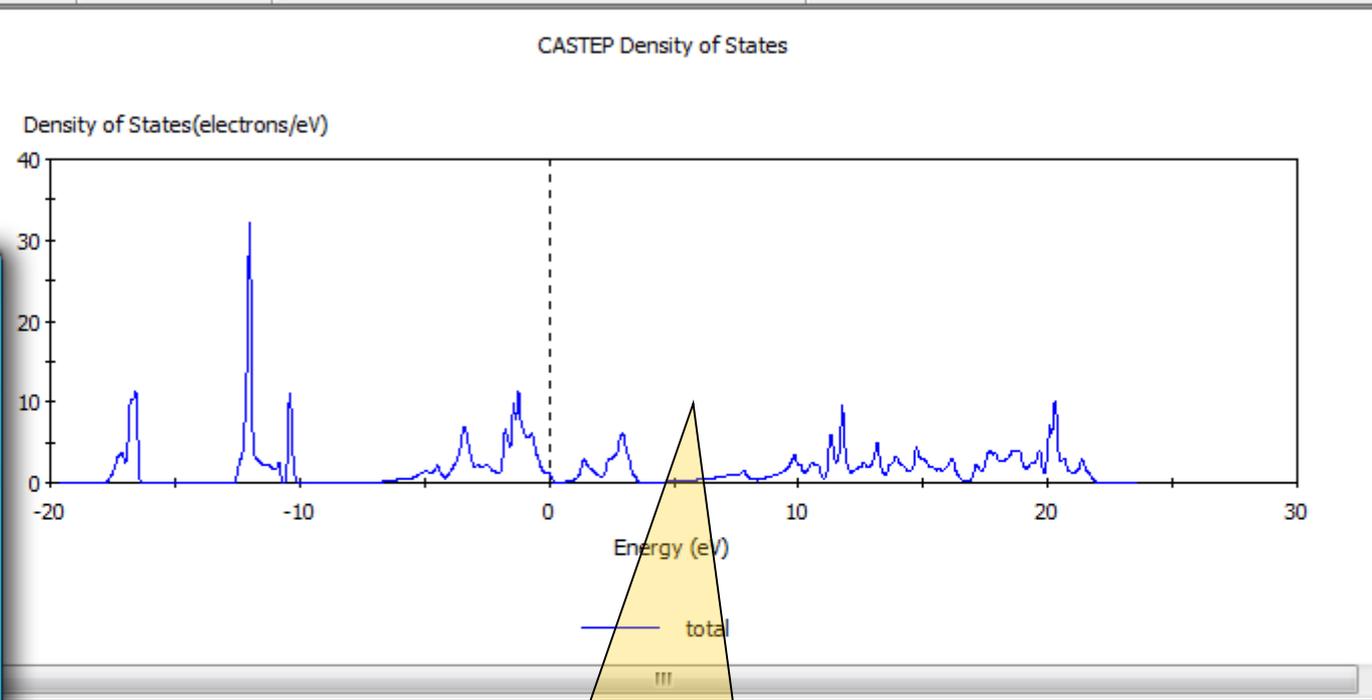
Function: DOS

Smoothing: 0.0 eV

Atom Selection

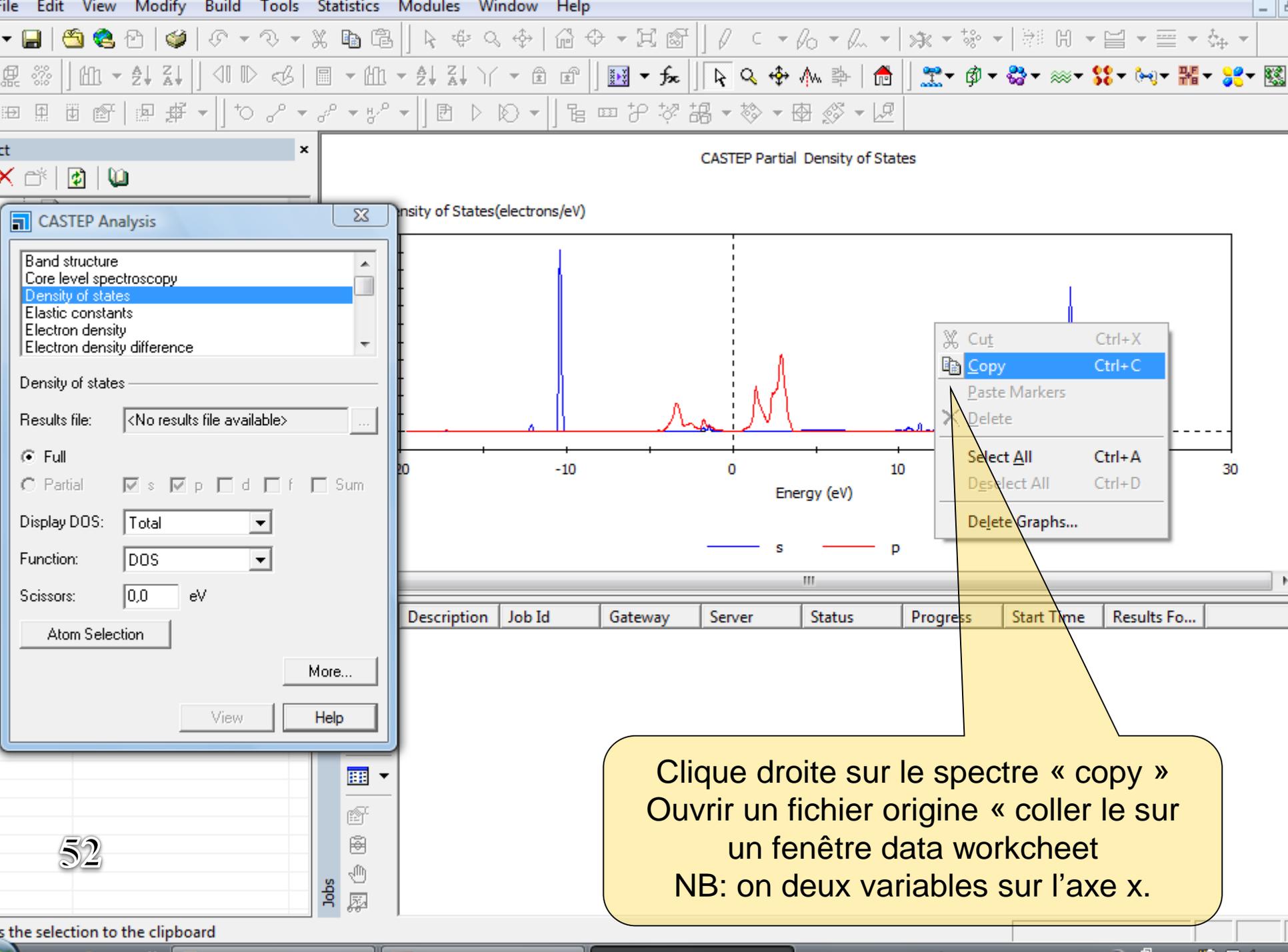
More...

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

- 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...
--------	---------	--------	--------	----------	------------	---------------

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 with the CASTEP Calculation tool open. The tool is configured for calculating elastic constants. The 'Setup' tab is active, showing the following settings:

- Task: Elastic Constants
- Quality: Customized
- Functional: GGA, PBE
- Spin polarized:
- Use formal spin as initial:
- Use LDA+U:
- Initial spin: 0
- Charge: 0

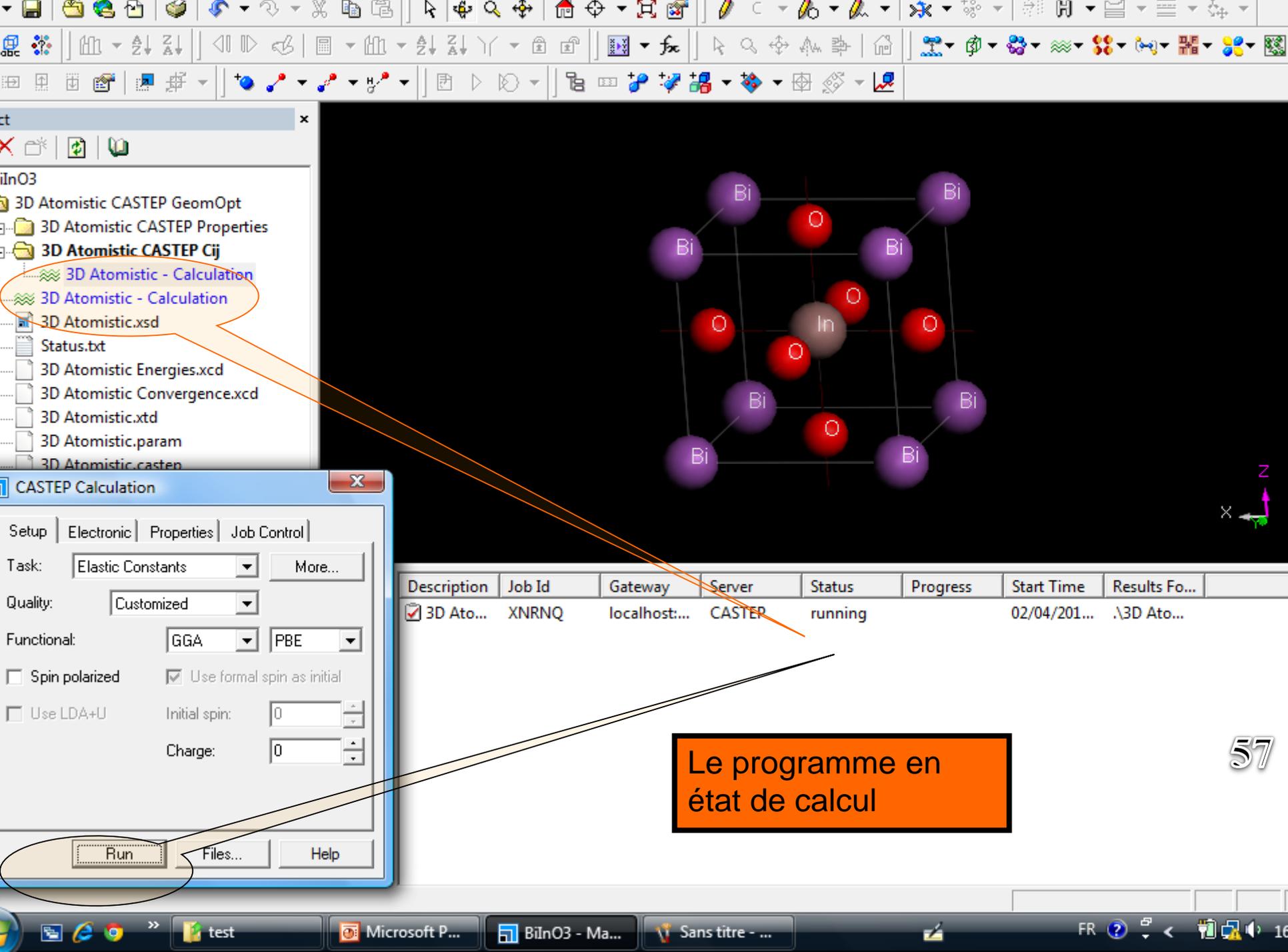
The 'CASTEP Elastic Constants' dialog is also open, showing the following settings:

- Elastic Constants | Options
- Number of steps for each strain: 6
- Maximum strain amplitude: 0.003
- Use volume-conserving strains:
- Strain pattern:

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

A yellow callout box points to the '3D Atomistic' folder in the Project tree, containing the text: 3D Atomisticdocument.xsd optimisé

Opens the CASTEP Calculation tool



File Explorer window showing a directory structure for a BiInO3 project. The file '3D Atomistic - Calculation' is circled in orange.

- BiInO3
 - 3D Atomistic CASTEP GeomOpt
 - 3D Atomistic CASTEP Properties
 - 3D Atomistic CASTEP Cij
 - 3D Atomistic - Calculation
 - 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

CASTEP Calculation dialog box. The 'Run' button is circled in orange.

Setup | Electronic | Properties | Job Control

Task: Elastic Constants [More...]

Quality: Customized

Functional: GGA [PBE]

Spin polarized Use formal spin as initial

Use LDA+U Initial spin: 0 Charge: 0

Run Files... Help

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

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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Copyright (c) 2000 - 2008

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

Properties

Filter:

Property	Value

Jobs

Fin de calcul
Des C_{ij}