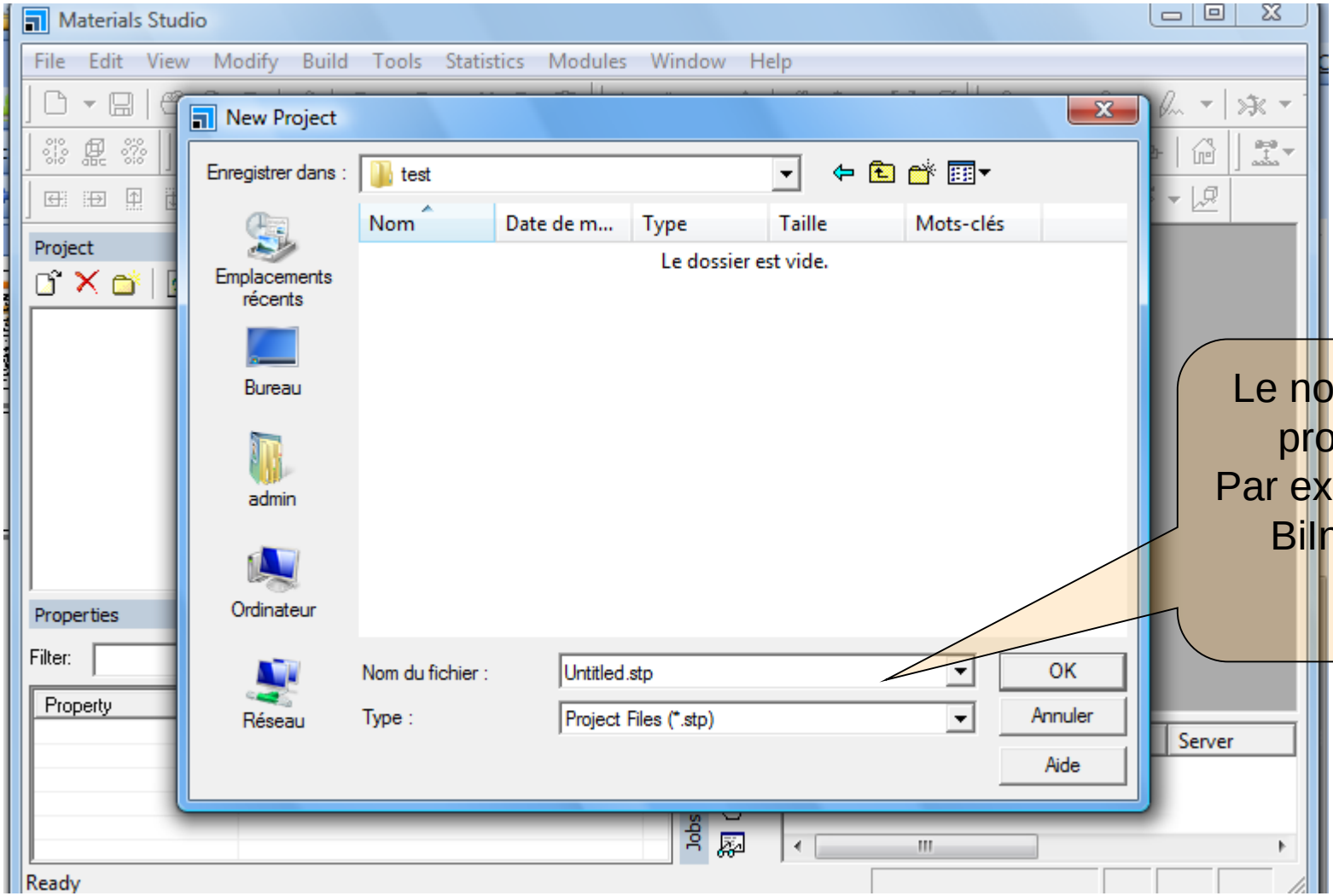
بسم الله الرحمن الرحيم

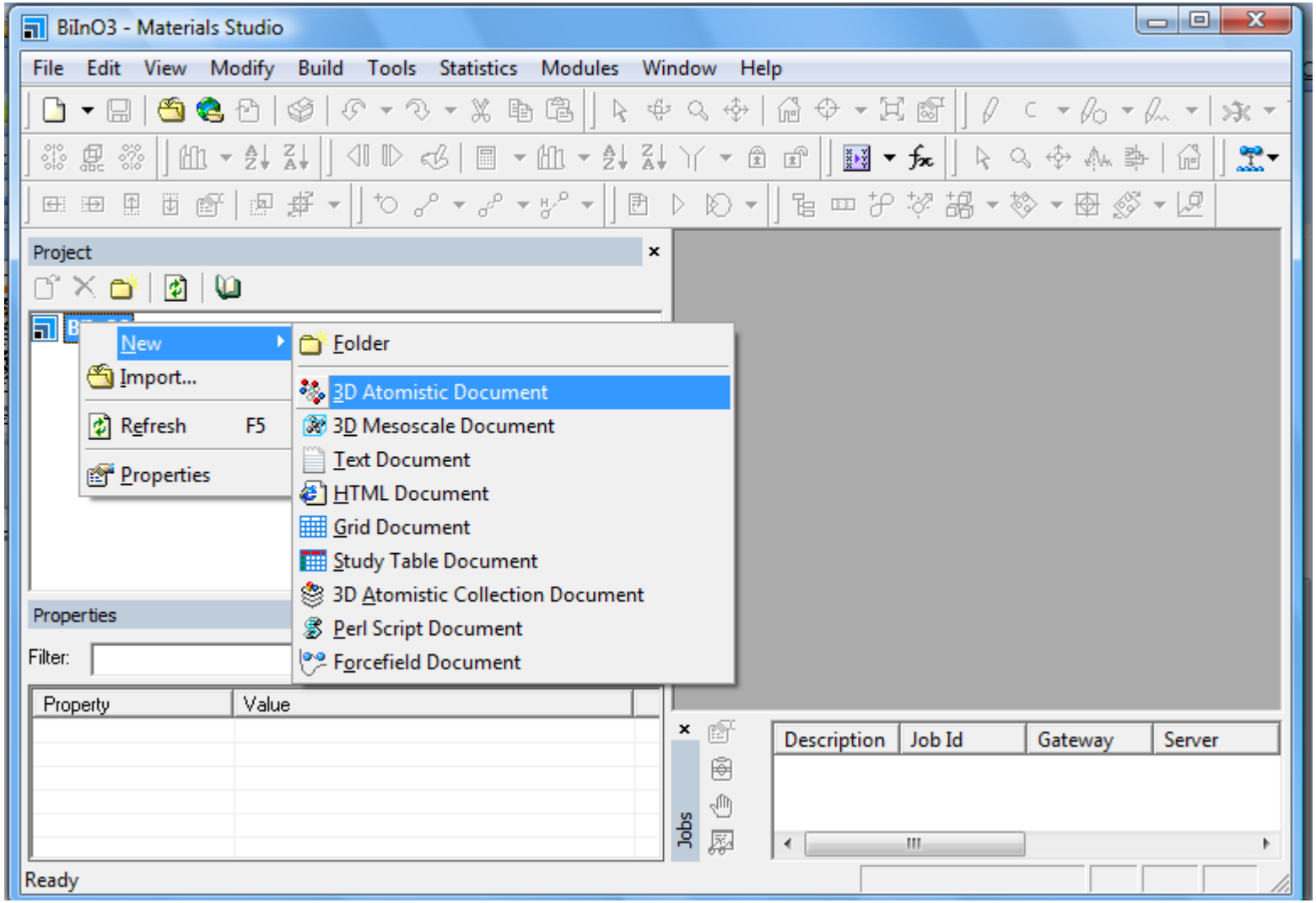
انشاء برنامج الحساب
CASTEP

Cambridge Sequential Total Energy Package

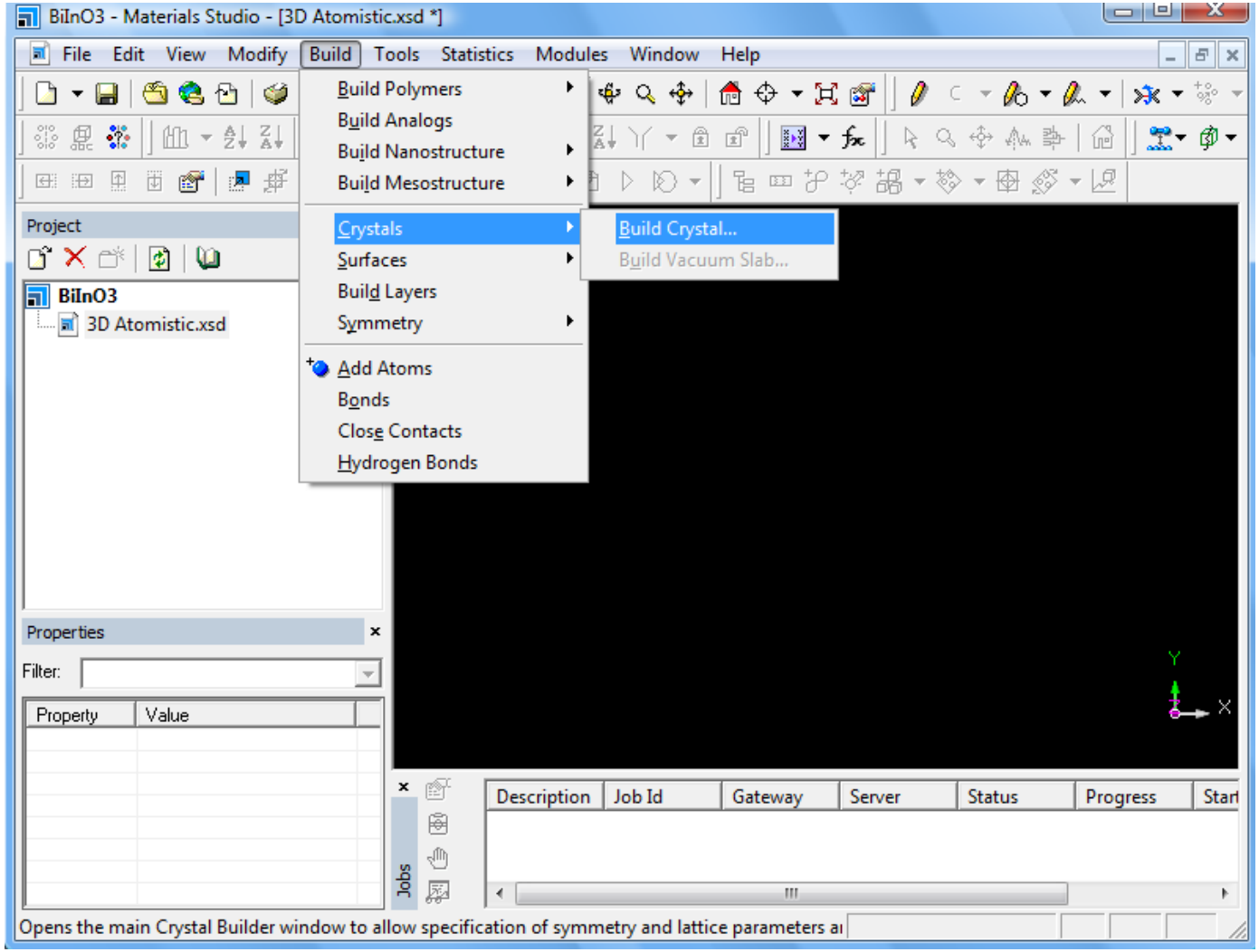
تفاصيل برنامج الحساب وتسمية مشروع الحساب تحت اسم المركب الذي نريد حسابه



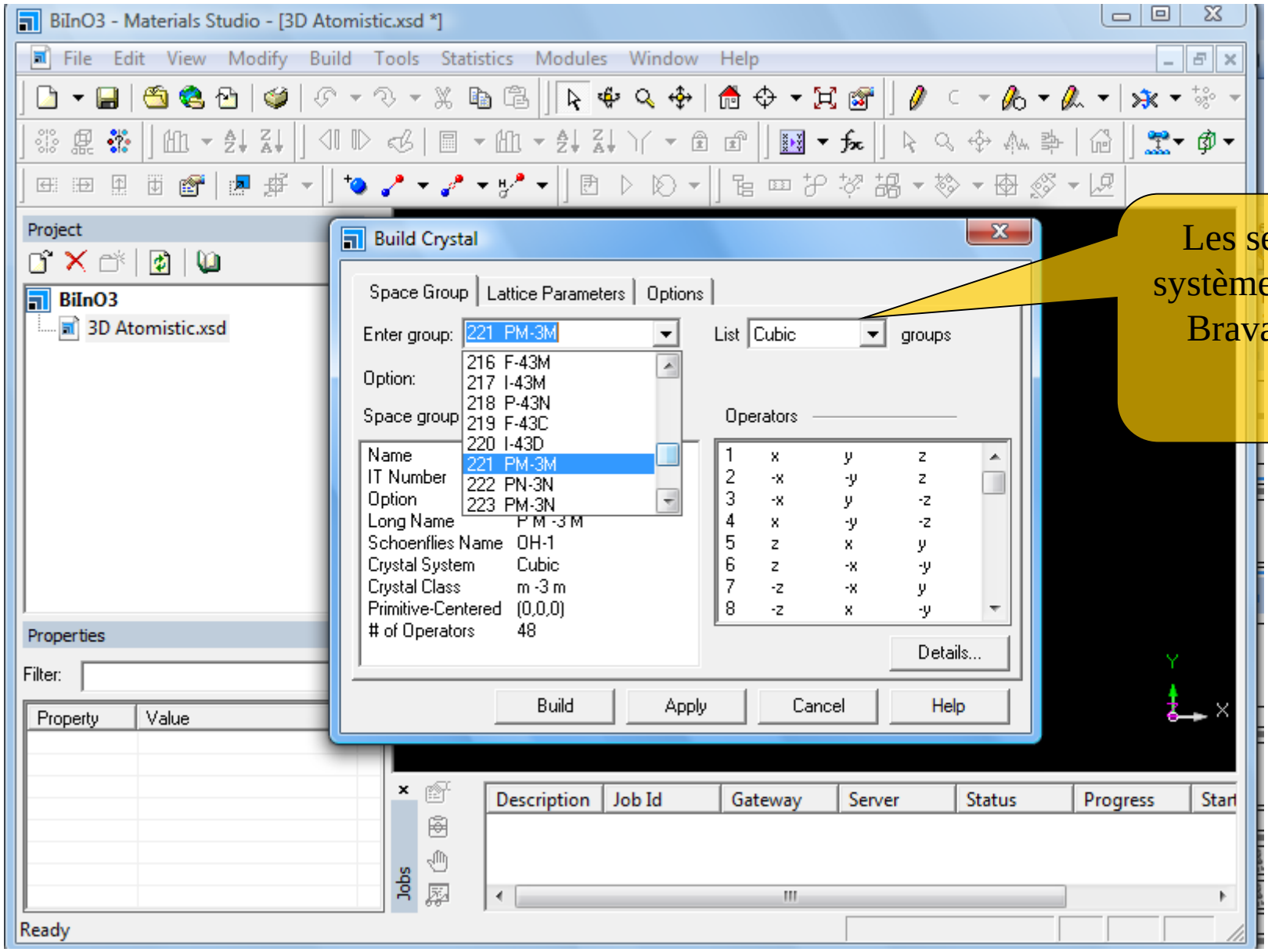
Une click droite de la sourie → New → 3D Atomistic Document



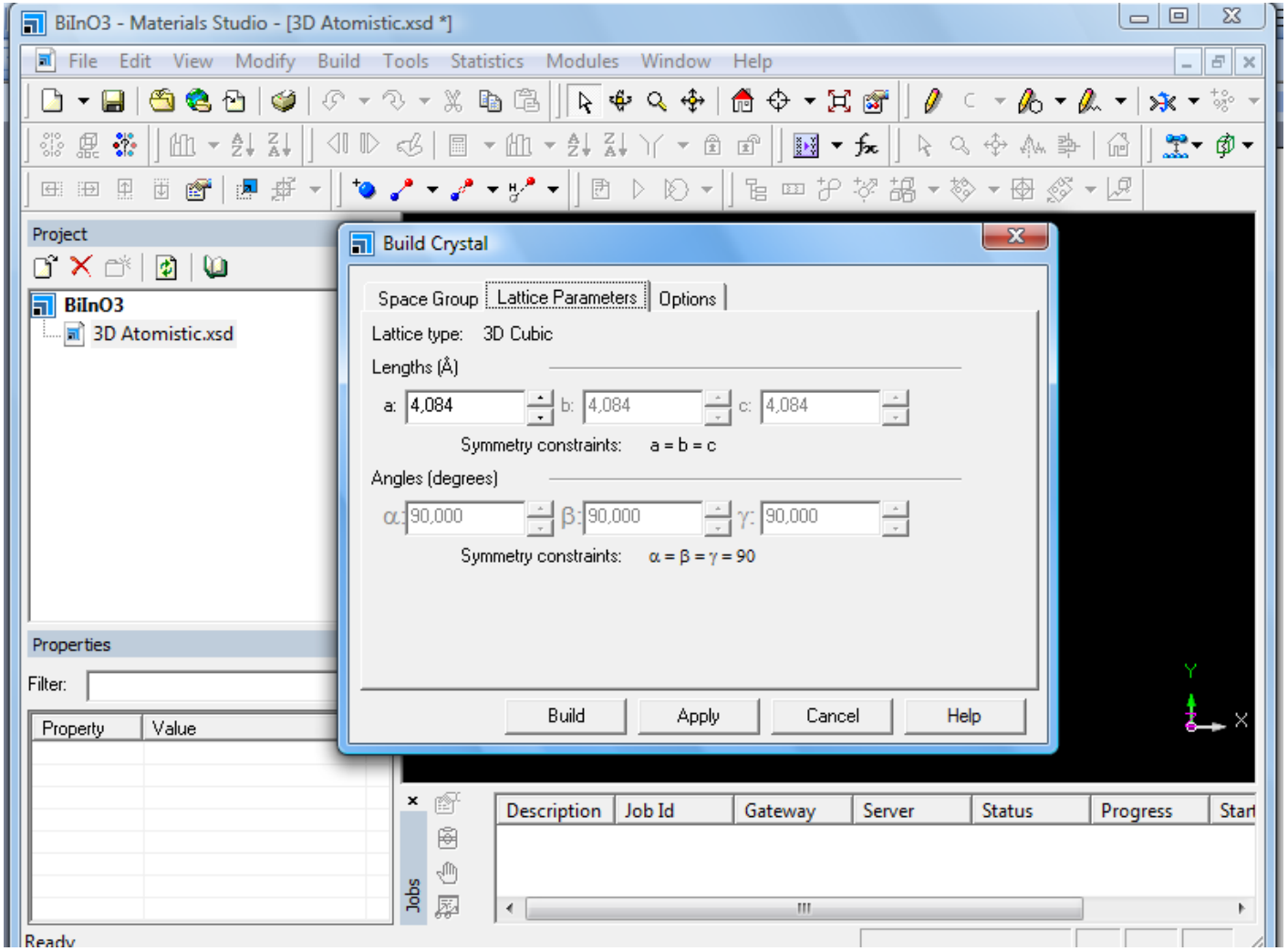
Appuyer sur Build → Crystals → Build crystal



Build Crystal → Space group → Choisir le groupe d'espace adéquat pour votre composé (MgAl2O4# 227)

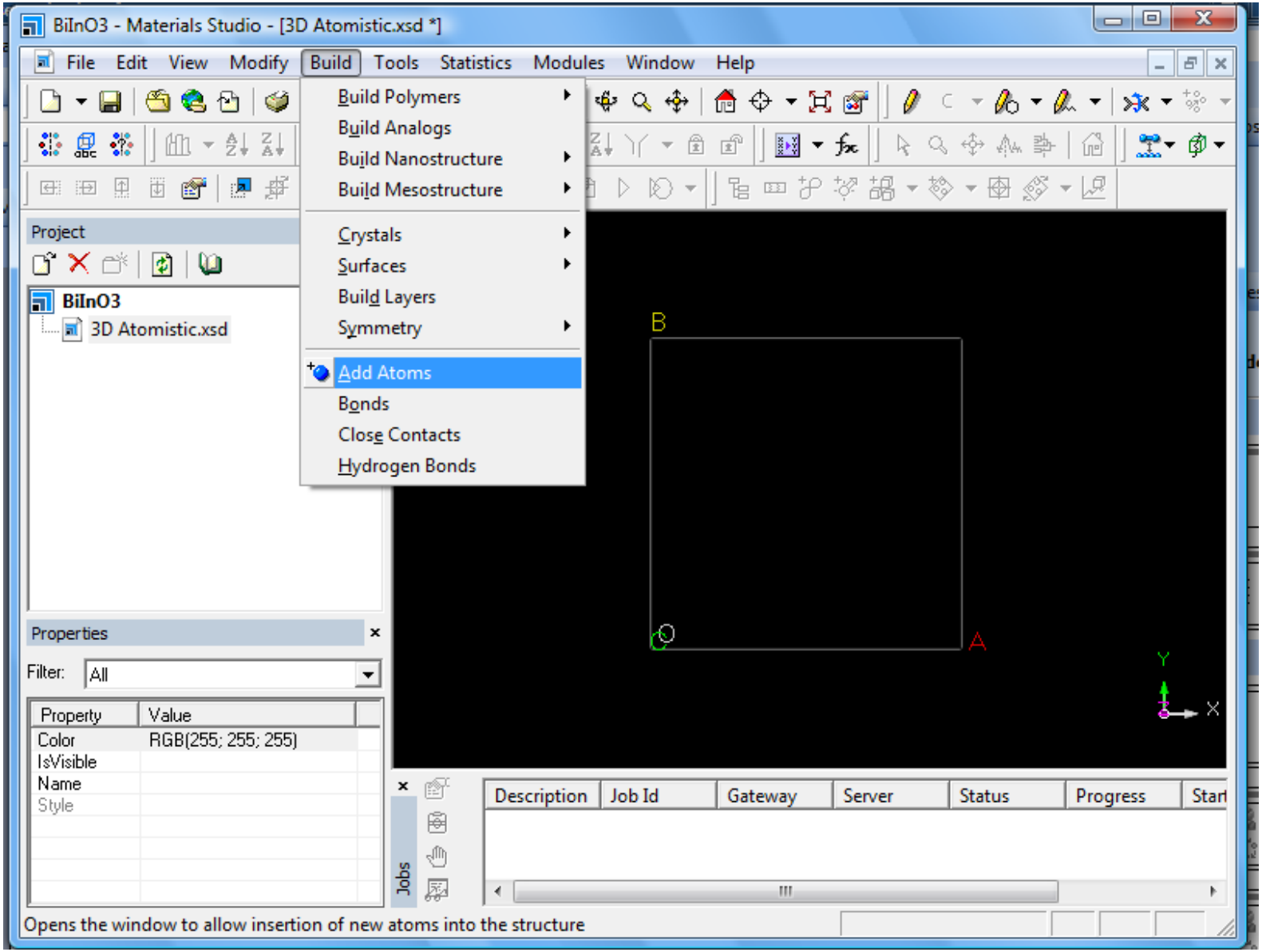


إدخال ثابت الشبكة البلورية

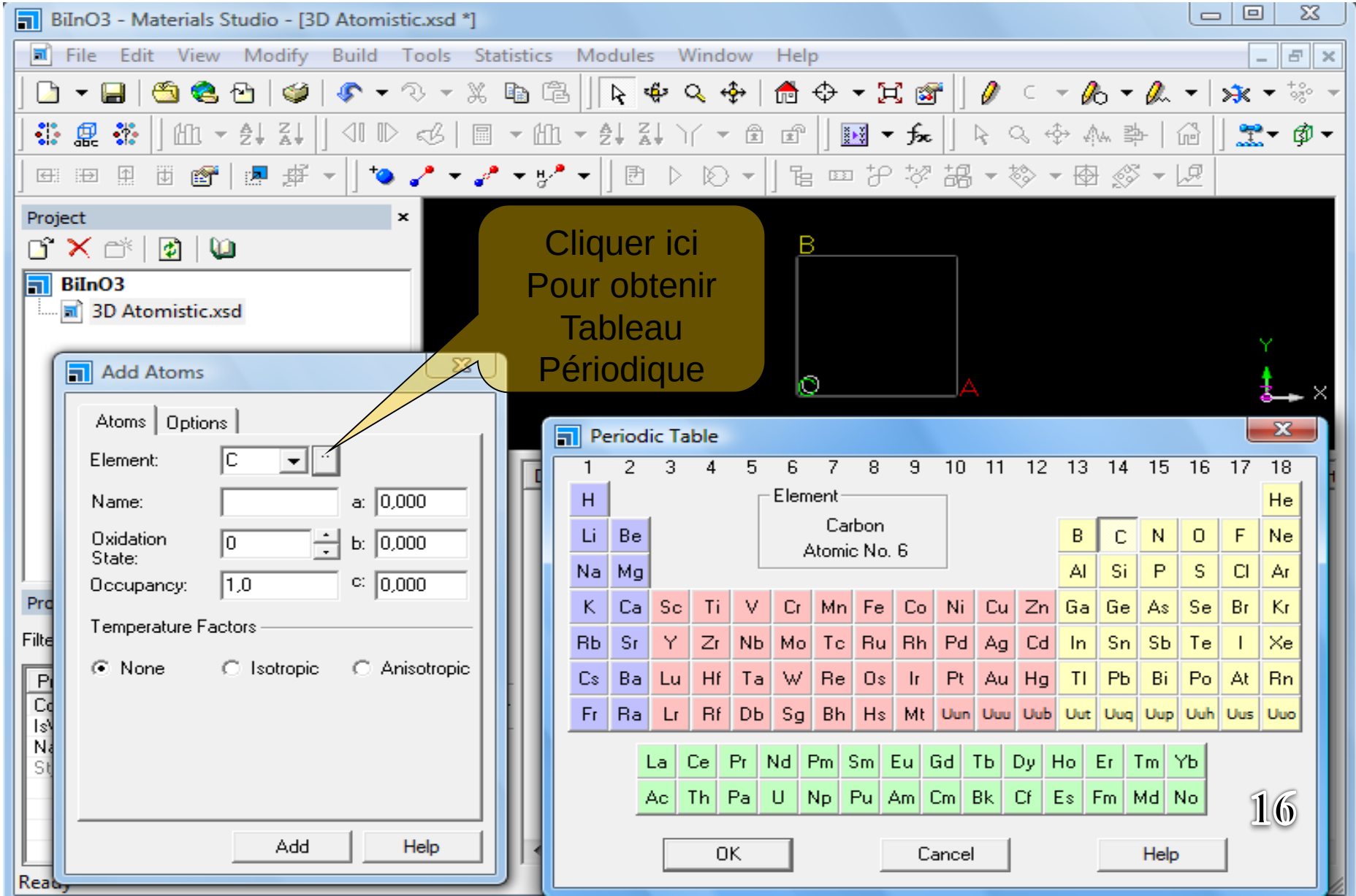


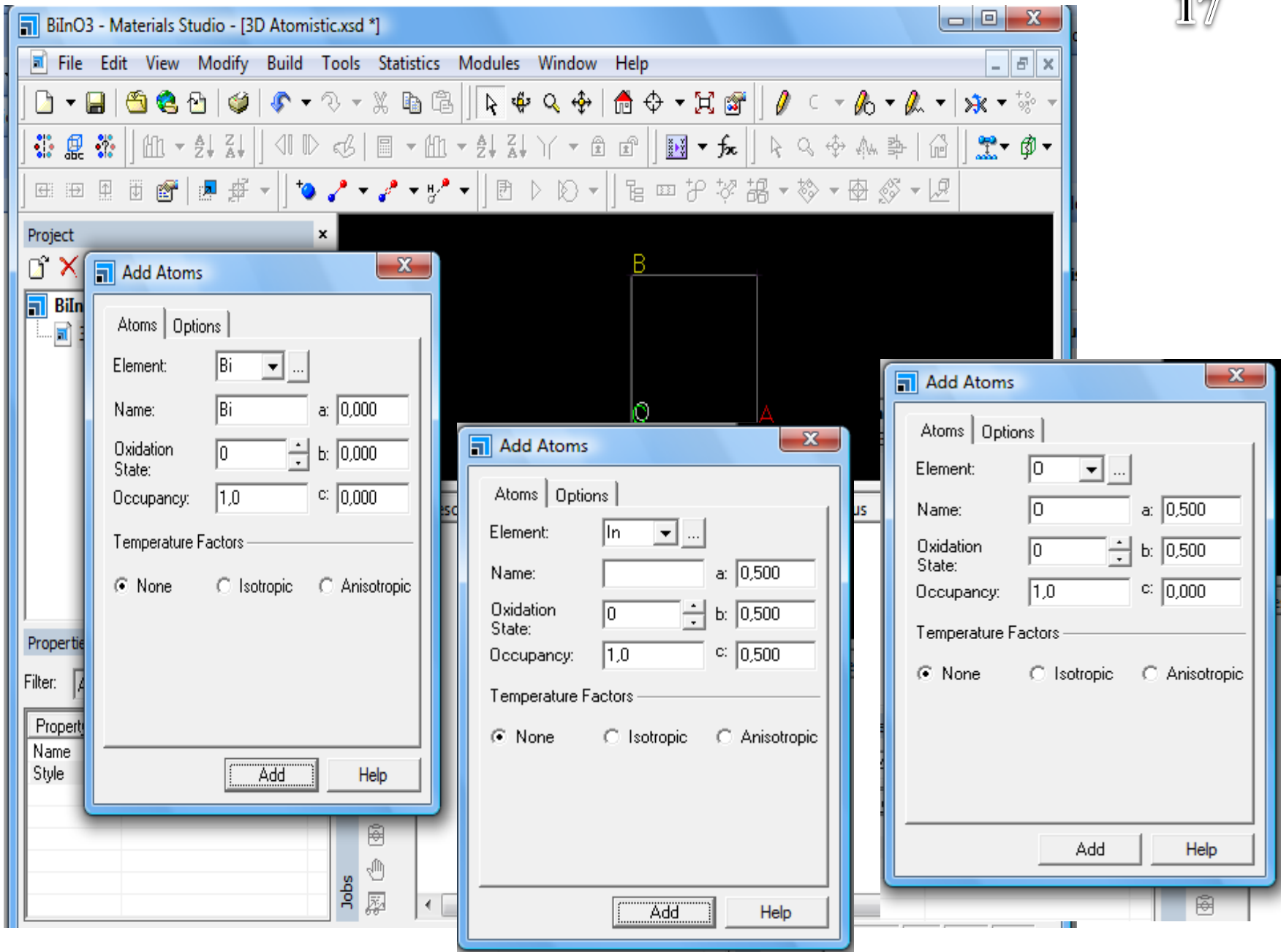
Pour chaque type de réseau de Bravais
Hexagonal, tetragonal, orthorhombique…..

إدخال احداثيات الذرات

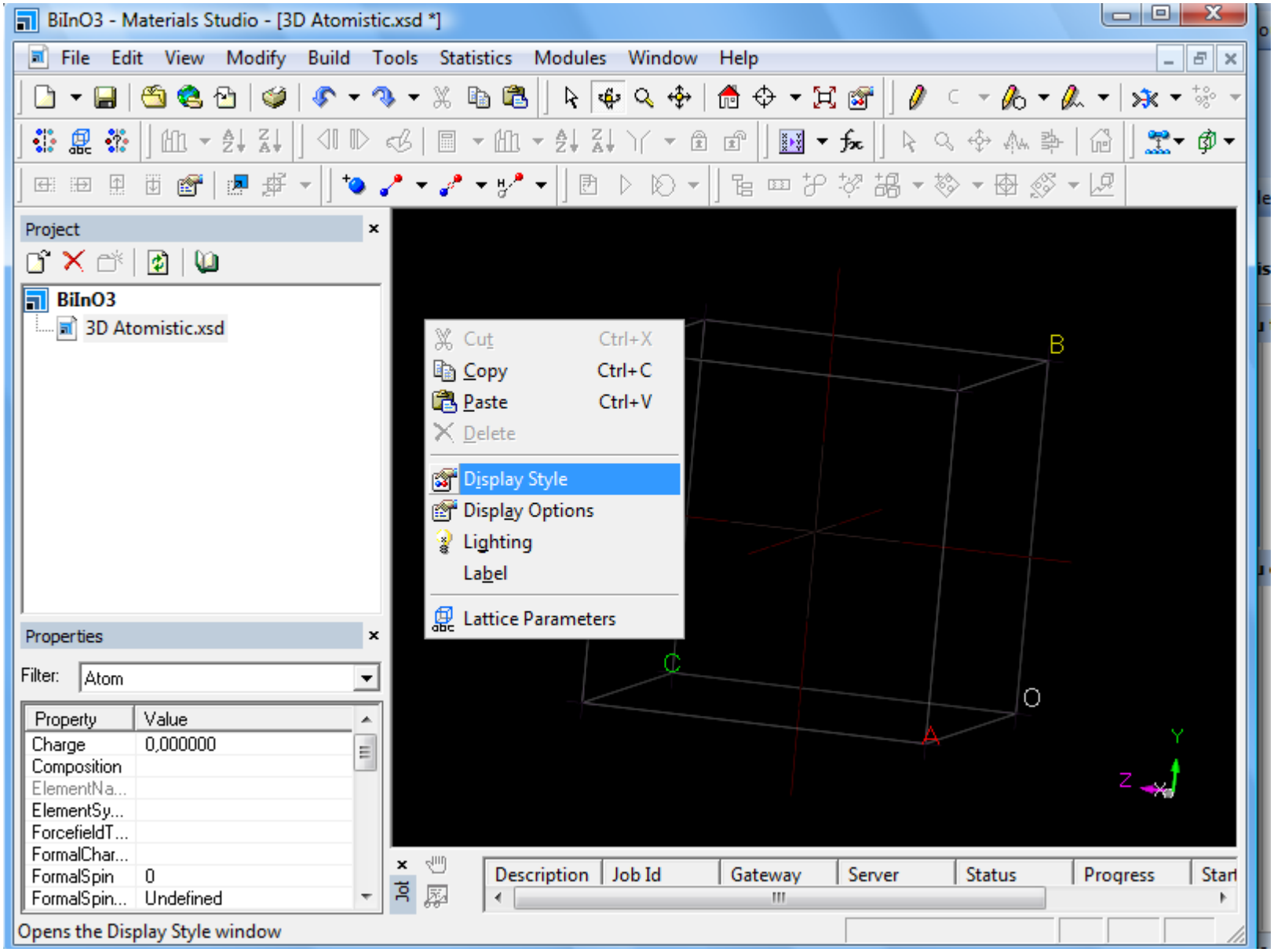


الضغط على العنصر الكيميائي ⟵ الجدول الدوري

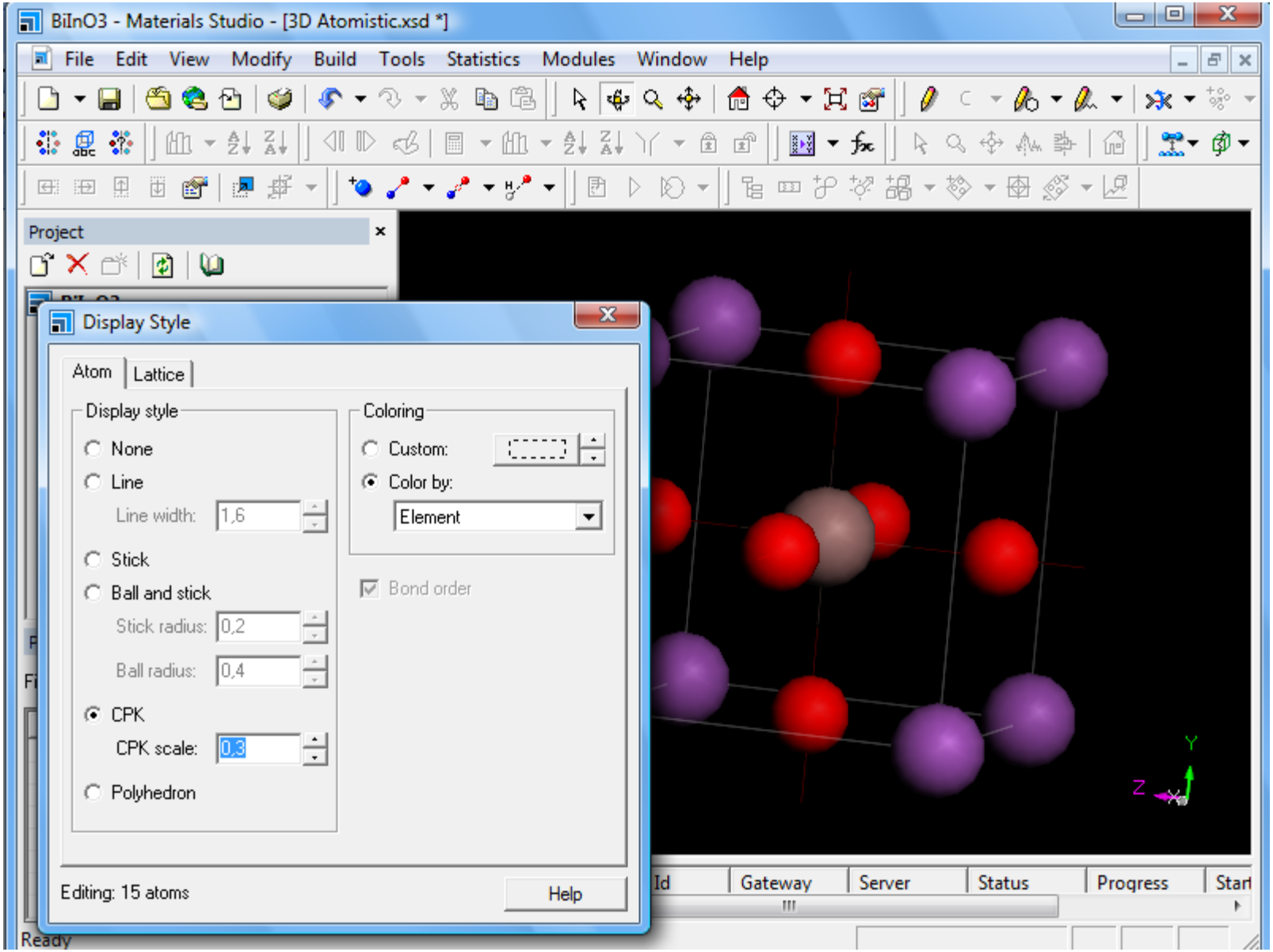



BiInO3 - Materials Studio - [3D Atomistic.xsd *]
File Edit View Modify Build Tools Statistics Modules Window Help
Project
B
O
A
Add Atoms
Atoms Options
Element: Bi
Name: Bi
a: 0,000
Oxidation State: 0
b: 0,000
Occupancy: 1,0
c: 0,000
Temperature Factors
None Isotropic Anisotropic
Add Help
Add Atoms
Atoms Options
Element: In
Name:
a: 0,500
Oxidation State: 0
b: 0,500
Occupancy: 1,0
c: 0,500
Temperature Factors
None Isotropic Anisotropic
Add Help
Add Atoms
Atoms Options
Element: O
Name: O
a: 0,500
Oxidation State: 0
b: 0,500
Occupancy: 1,0
c: 0,000
Temperature Factors
None Isotropic Anisotropic
Add Help
Filter:
Name
Style
Jobs

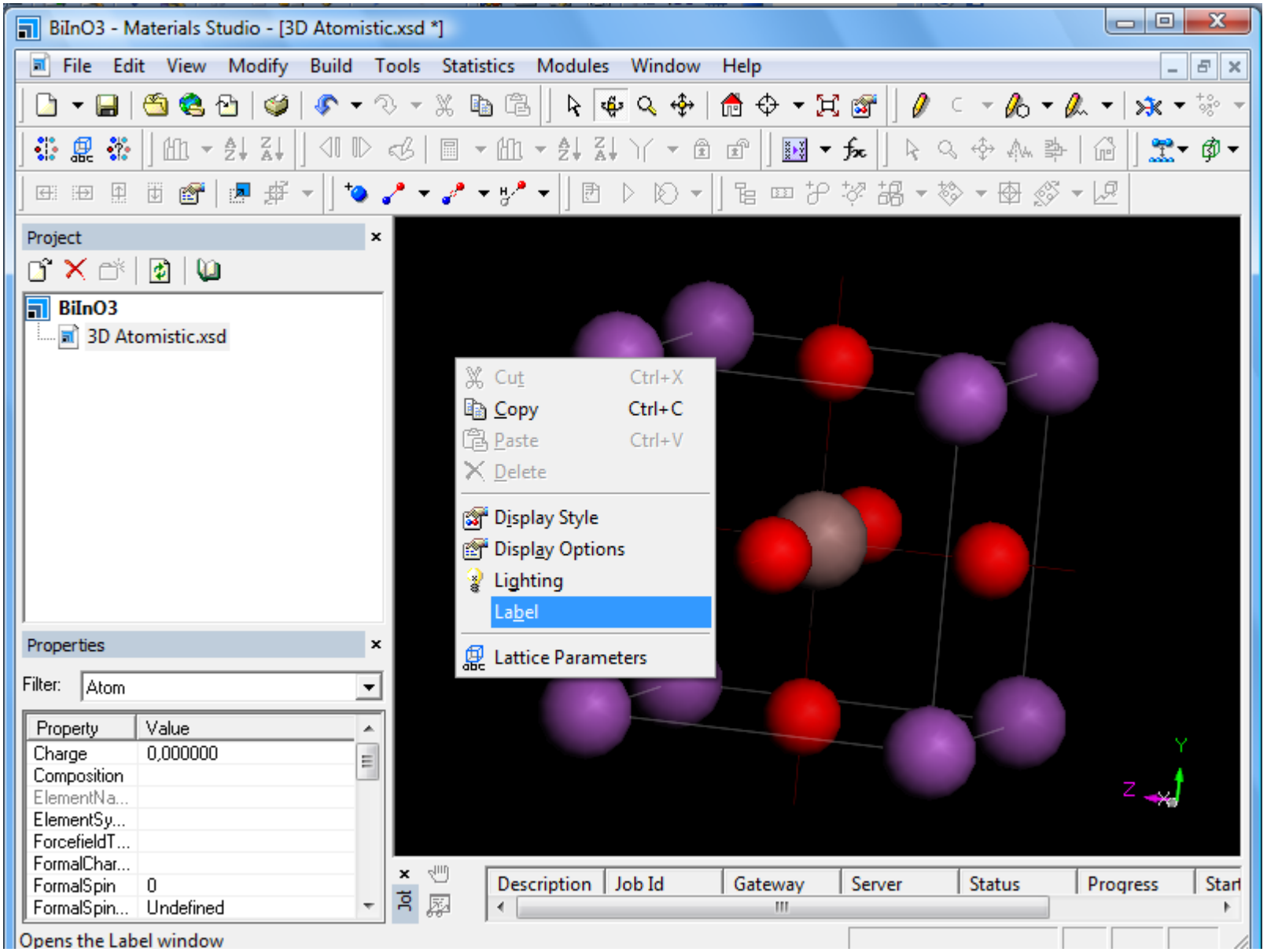
Clique droite ⟶ Display style ⟶ pour rendre les atomes sous forme sphérique



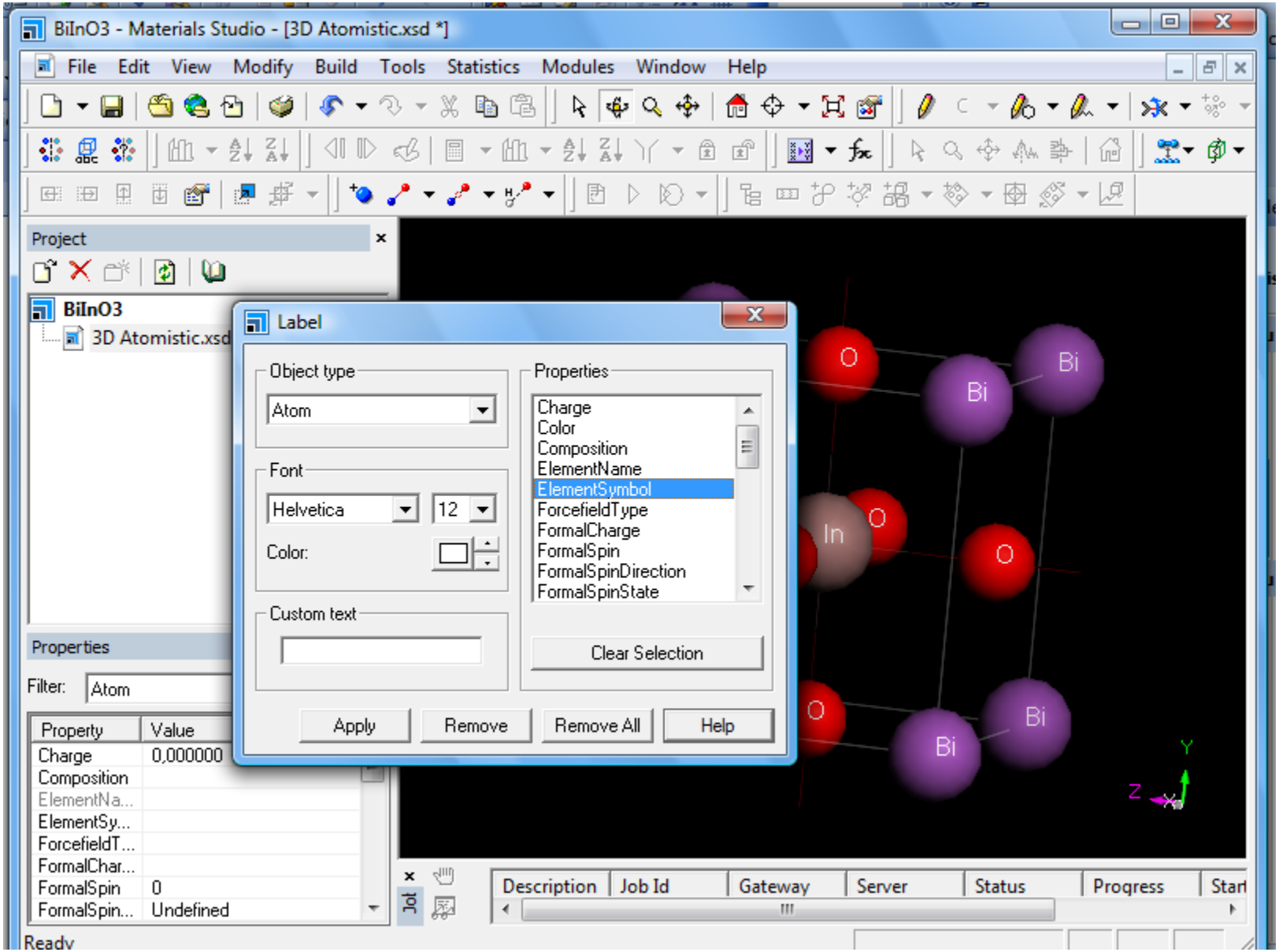
Display style ⟶ CPK ou Poyhedron ou bien Ball and Stick ⟶ en même temps vous pouvez choisir les options pour Lattice.



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

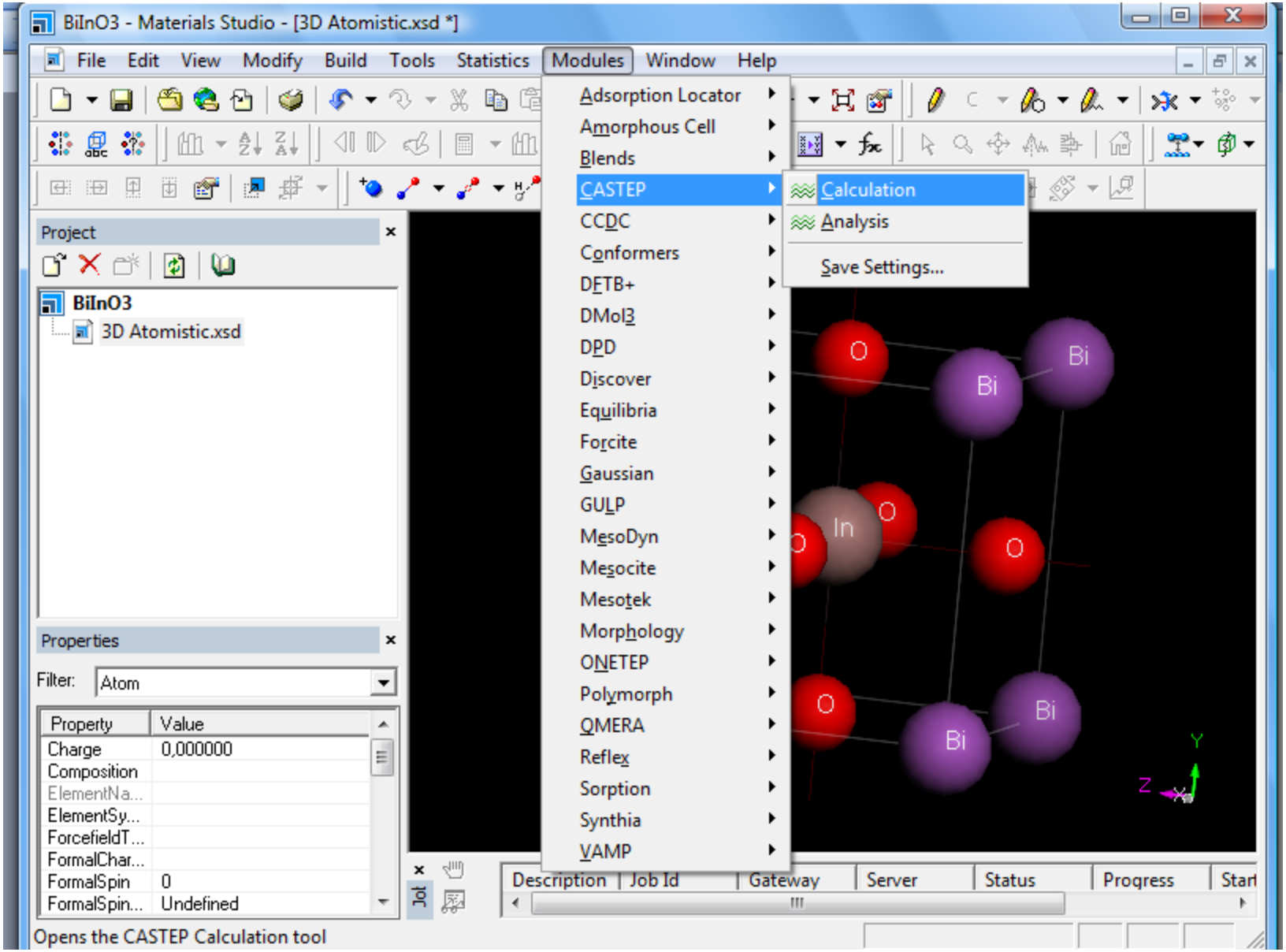


Plusieurs propriétés affichées soit ce qui concerne « Atom » ou bien « Bond »

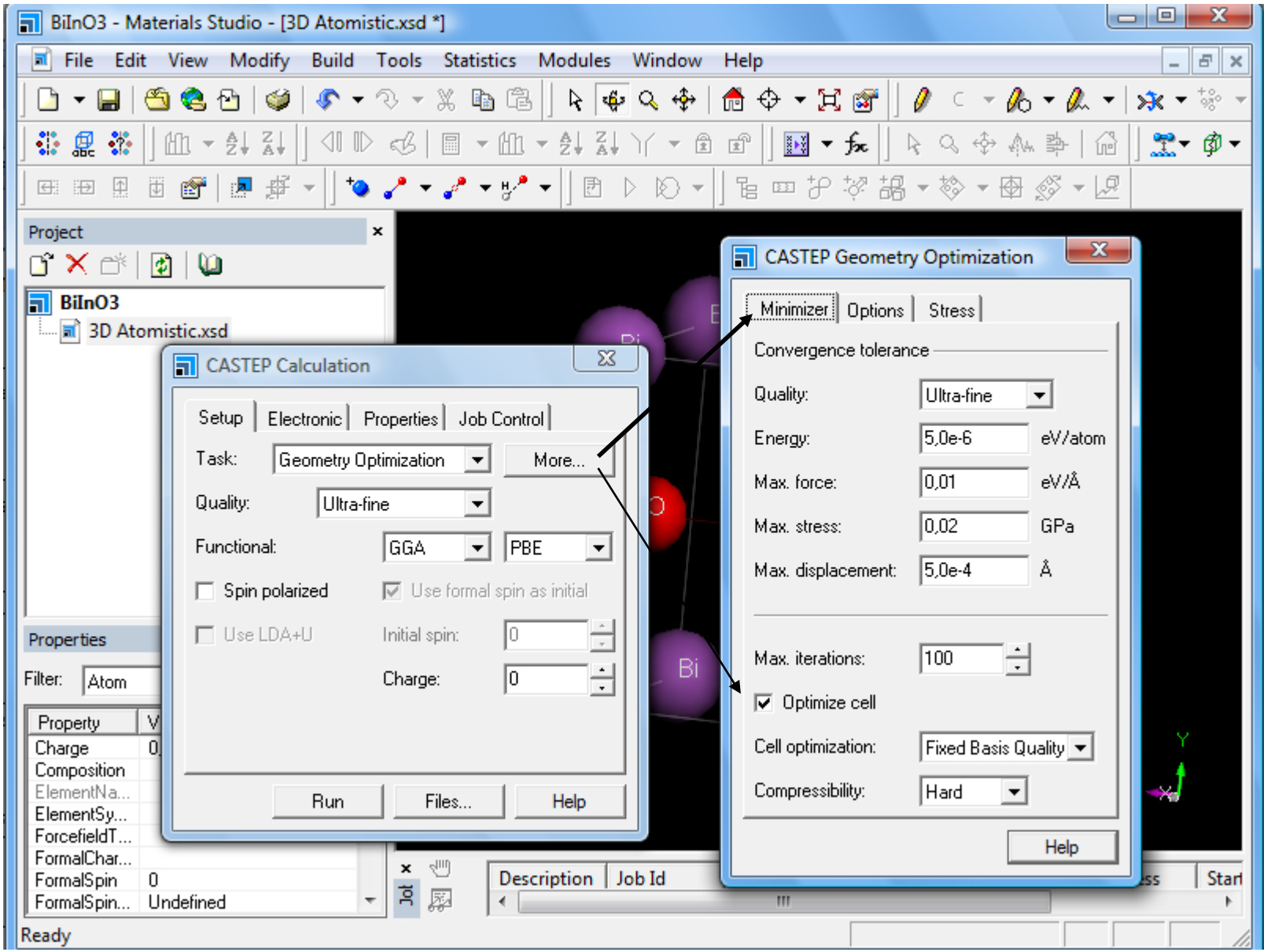


كيفية استعمال البرنامج الحسابي
le code CASTEP.

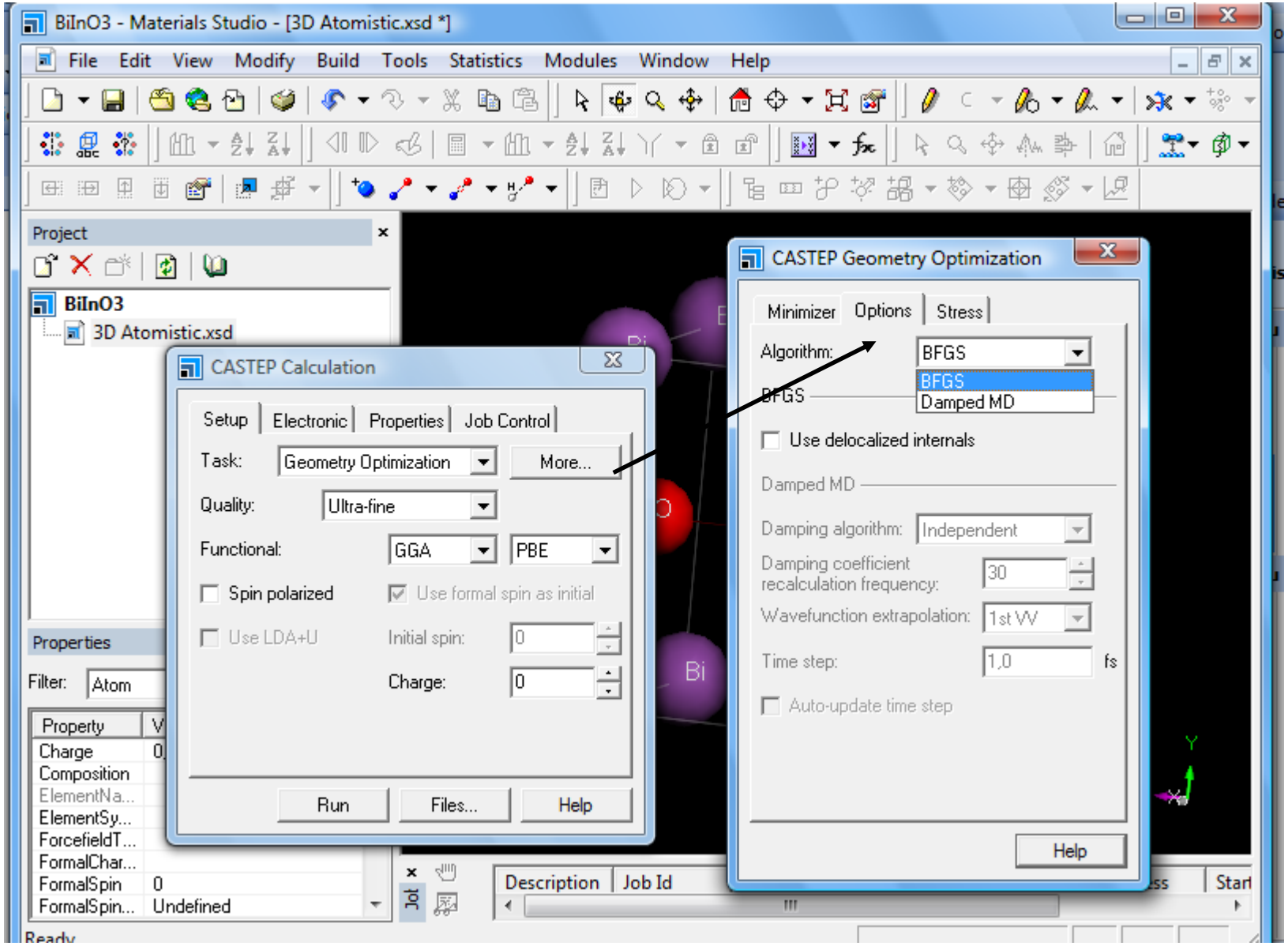
Modules → CASTEP → Calculation



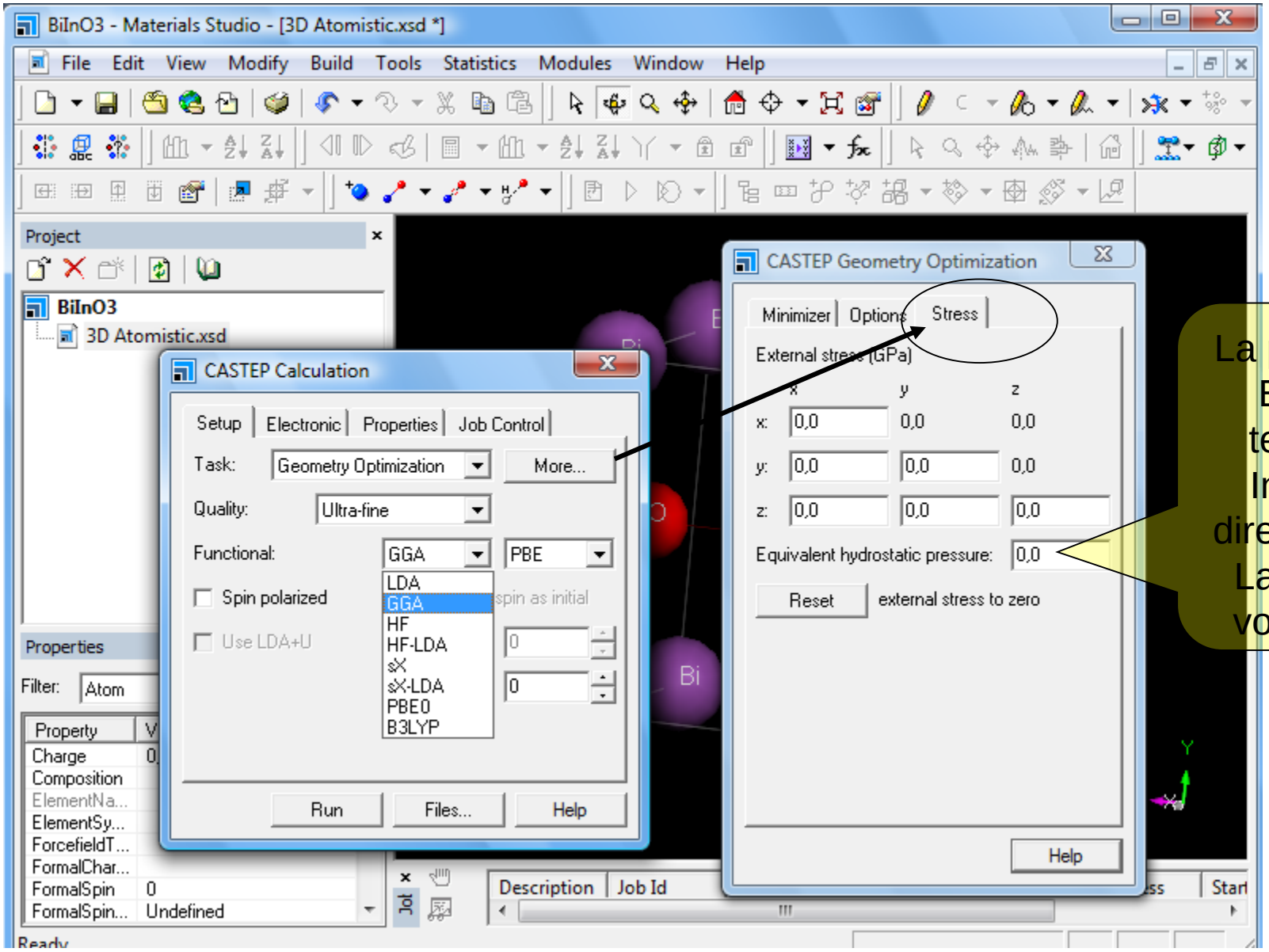
Task ⟶ geometry optimization ⟶ Minimizer ⟶ coucher optimize cell



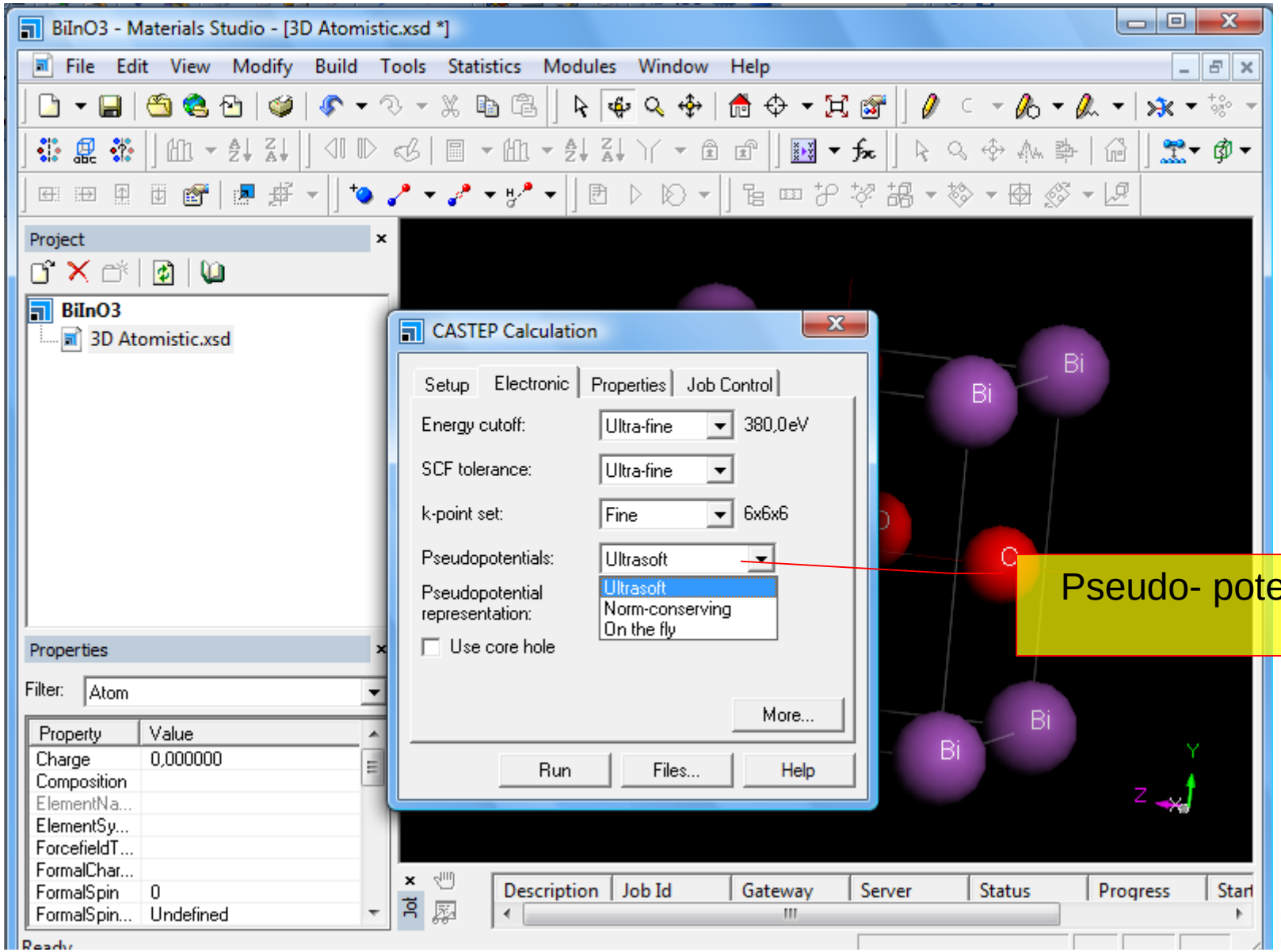
Task ⟶ geometry optimization ⟶ more et choisir l'algorithme voulu



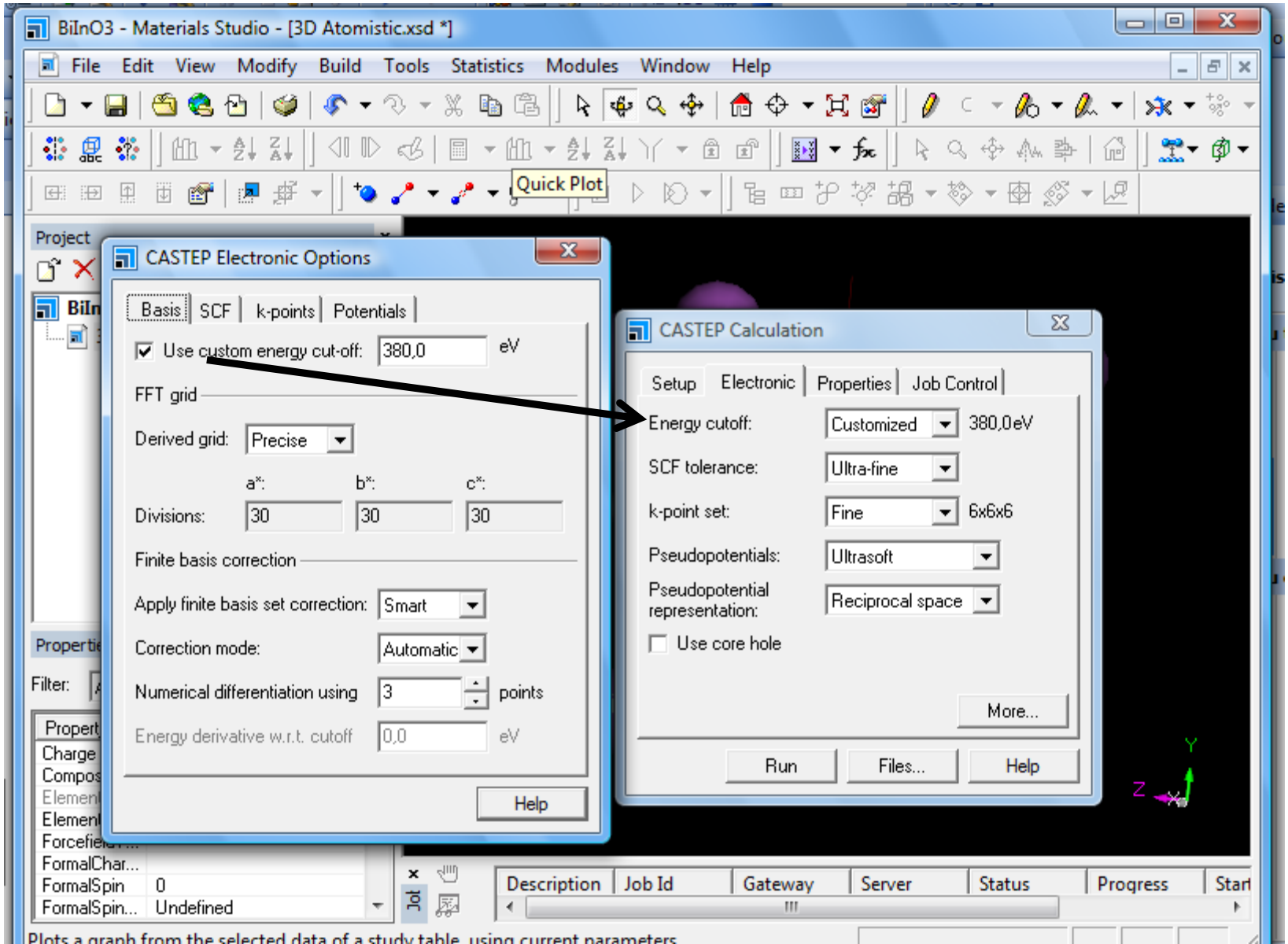
Cette tache nous permet de introduire la valeur du pression hydrostatique

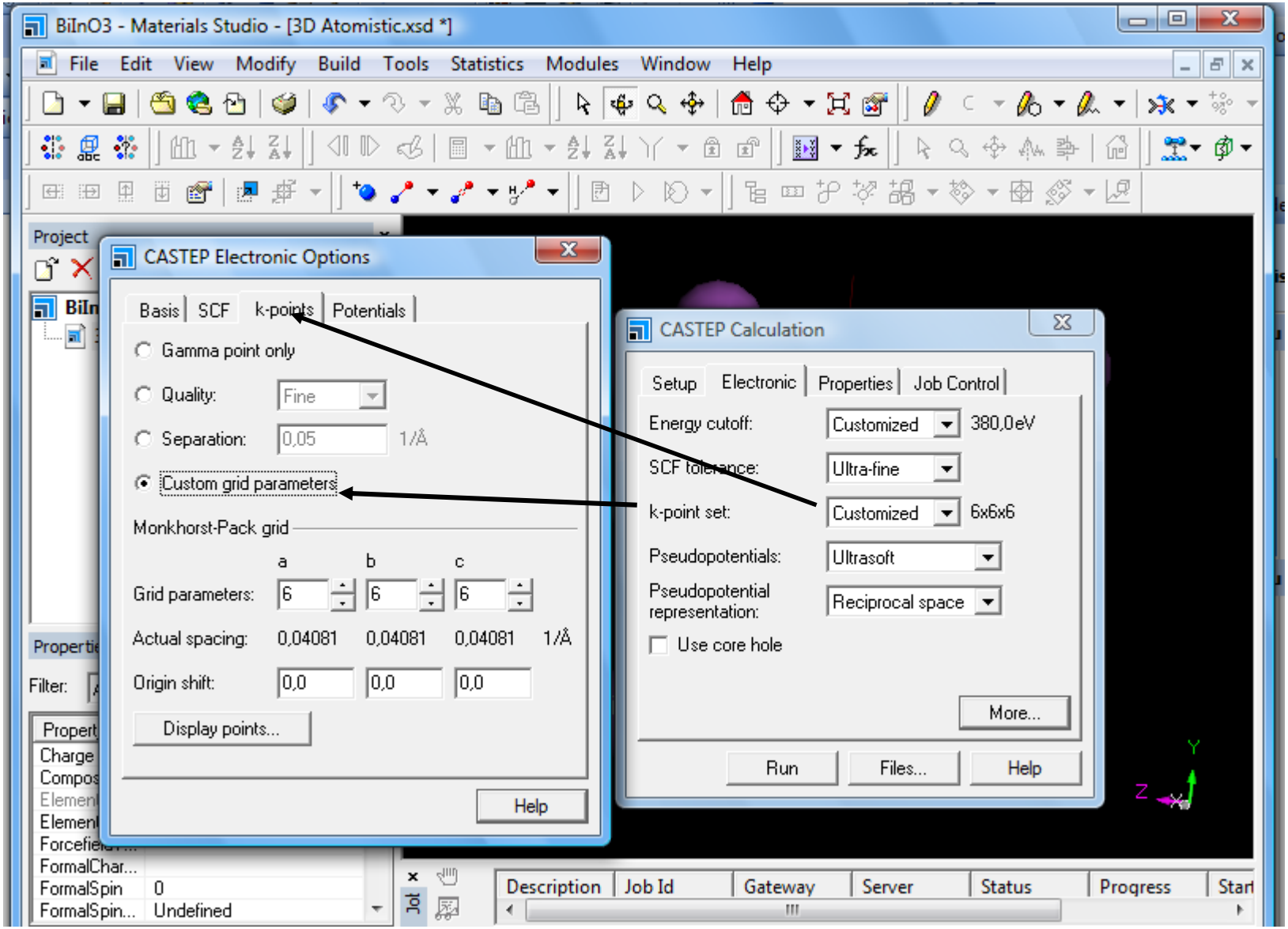


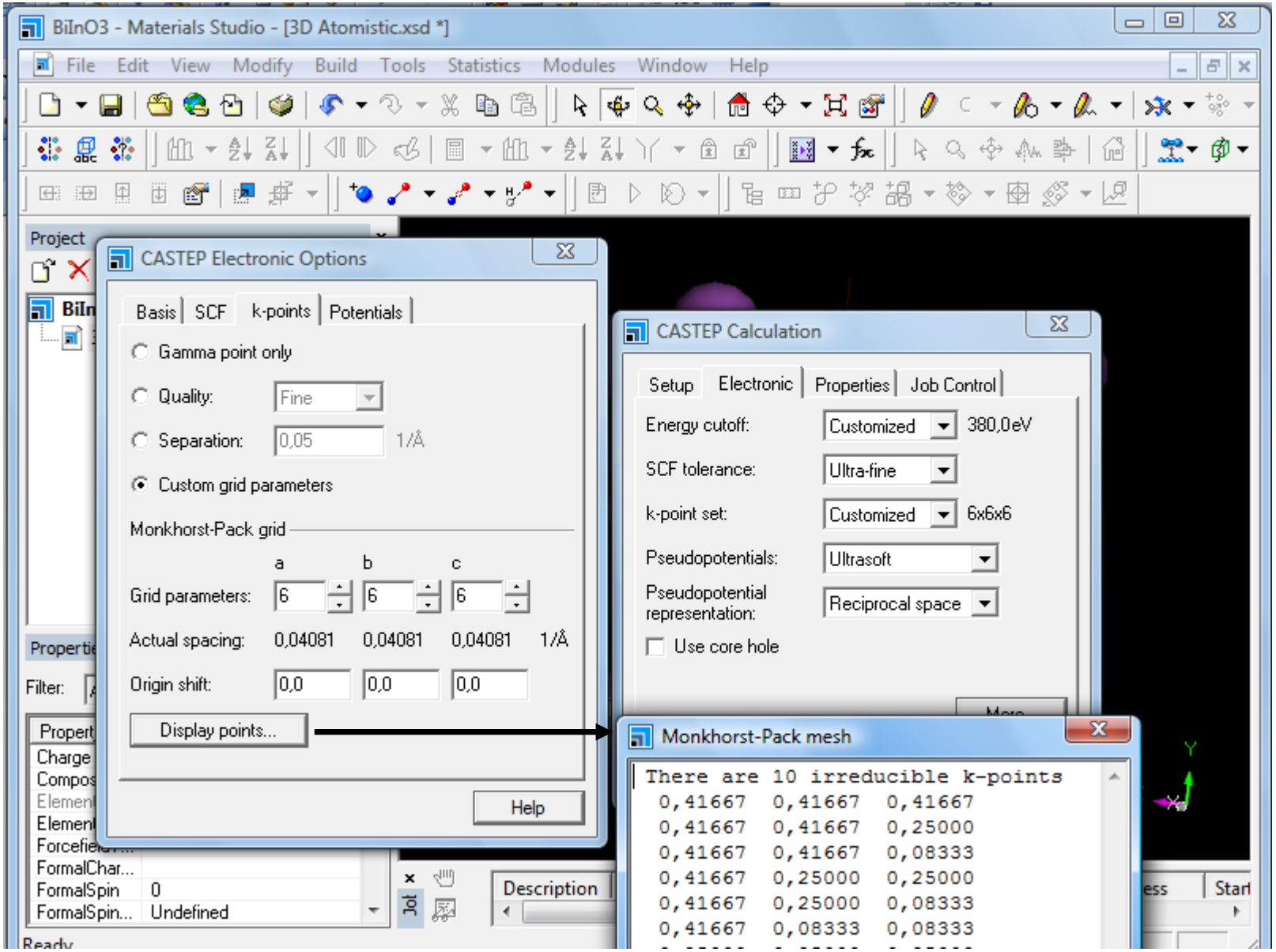
La pression
Est un
tenseur
Injecter
directement
La valeur
voulue ici


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 380,0eV
SCF tolerance: Ultra-fine
k-point set: Fine 6x6x6
Pseudopotentials: Ultrasoft
Pseudopotential representation:
Ultrasoft
Norm-conserving
On the fly
Use core hole
More...
Run Files... Help
Bi
C
Y
Z
Description Job Id Gateway Server Status Progress
Pseudo- potentiel

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

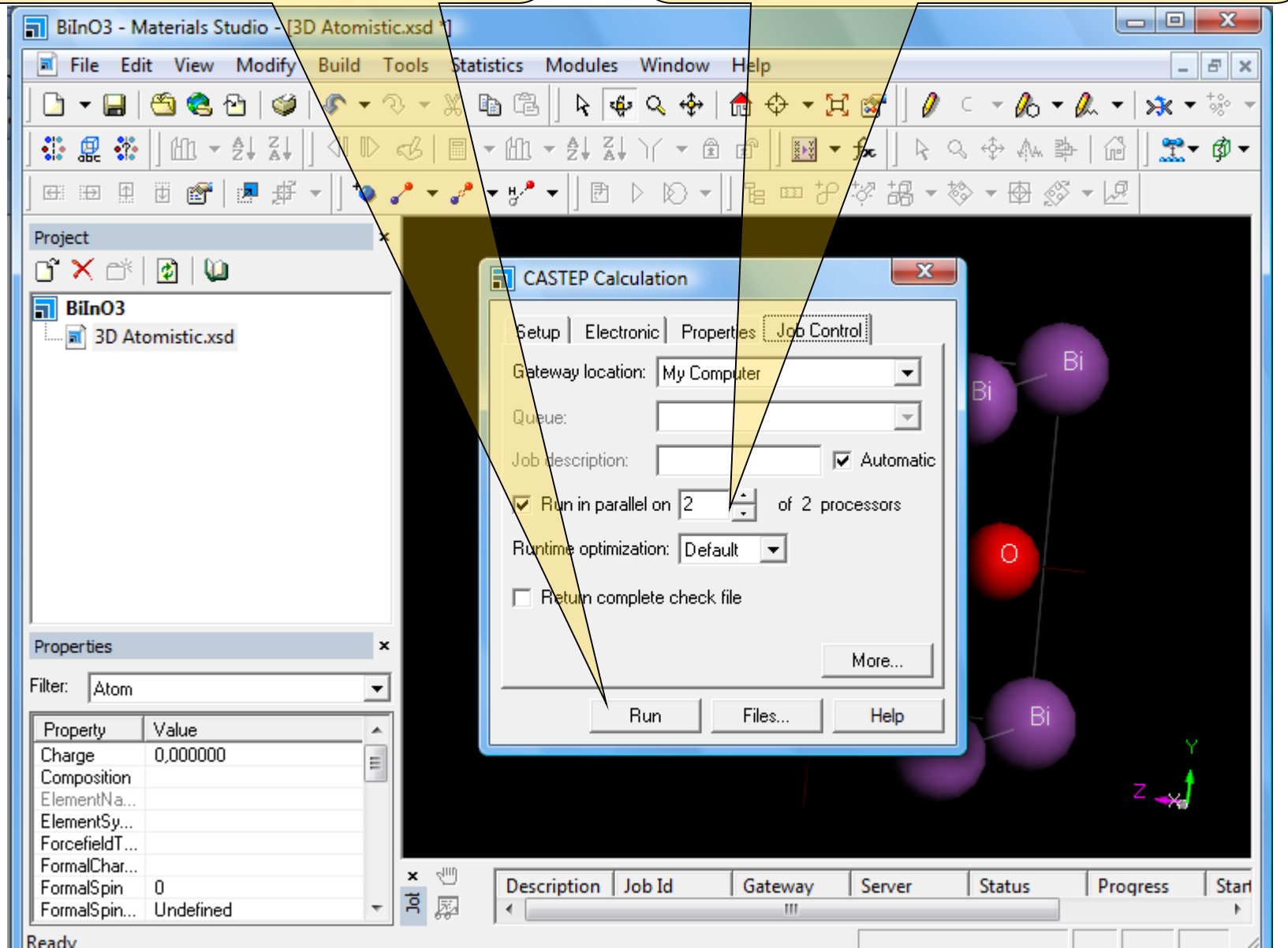


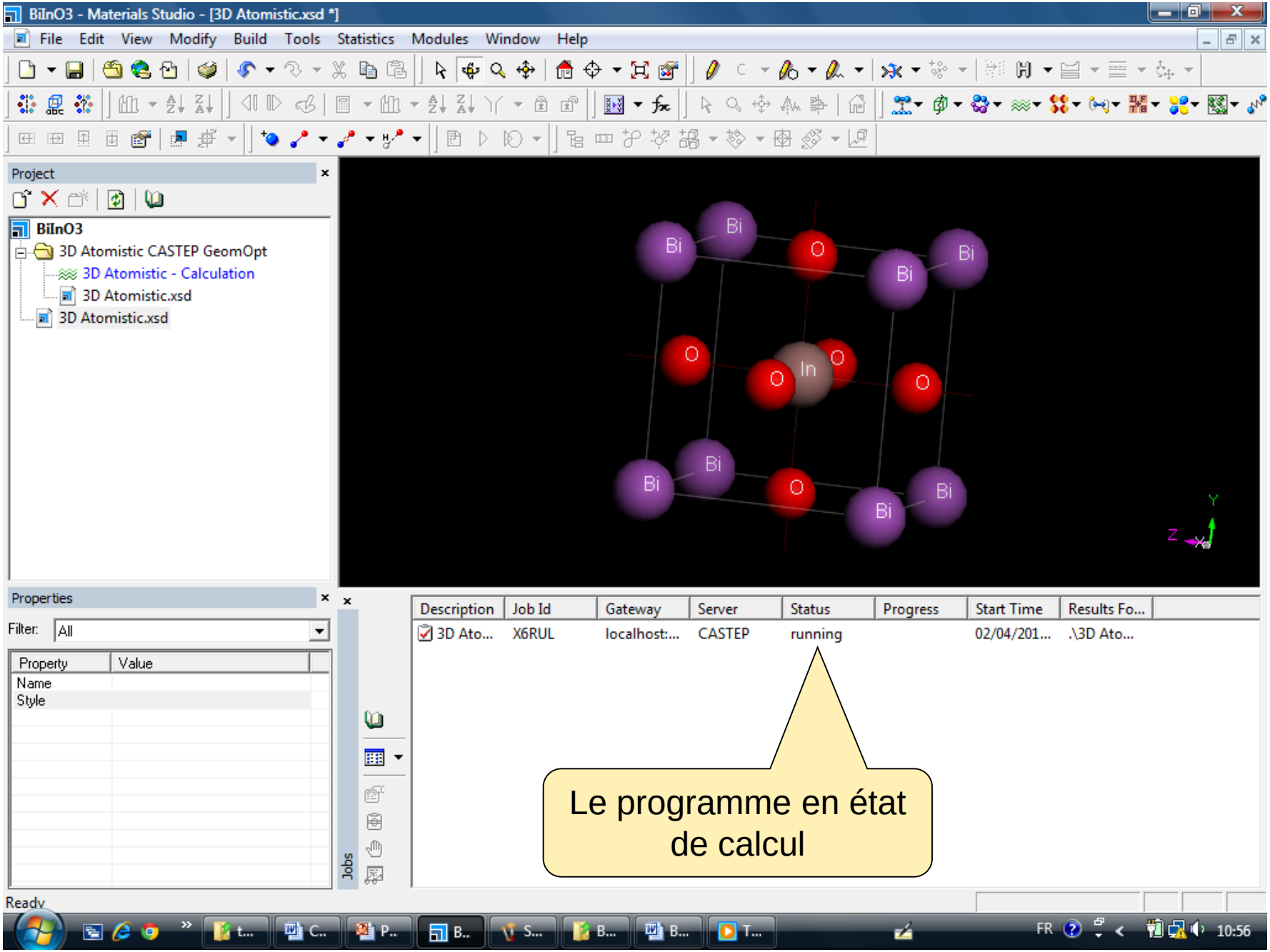

BiInO3 - Materials Studio - [3D Atomistic.xsd *]
File Edit View Modify Build Tools Statistics Modules Window Help
Project
CASTEP Electronic Options
Basis SCF k-points Potentials
Gamma point only
Quality: Fine
Separation: 0,05 1/Å
Custom grid parameters
Monkhorst-Pack grid
a b c
Grid parameters: 6 6 6
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
Filter:
Charge
FormalChar...
FormalSpin 0
FormalSpin... Undefined
Description Job Id Gateway Server Status Progress
Y
Z

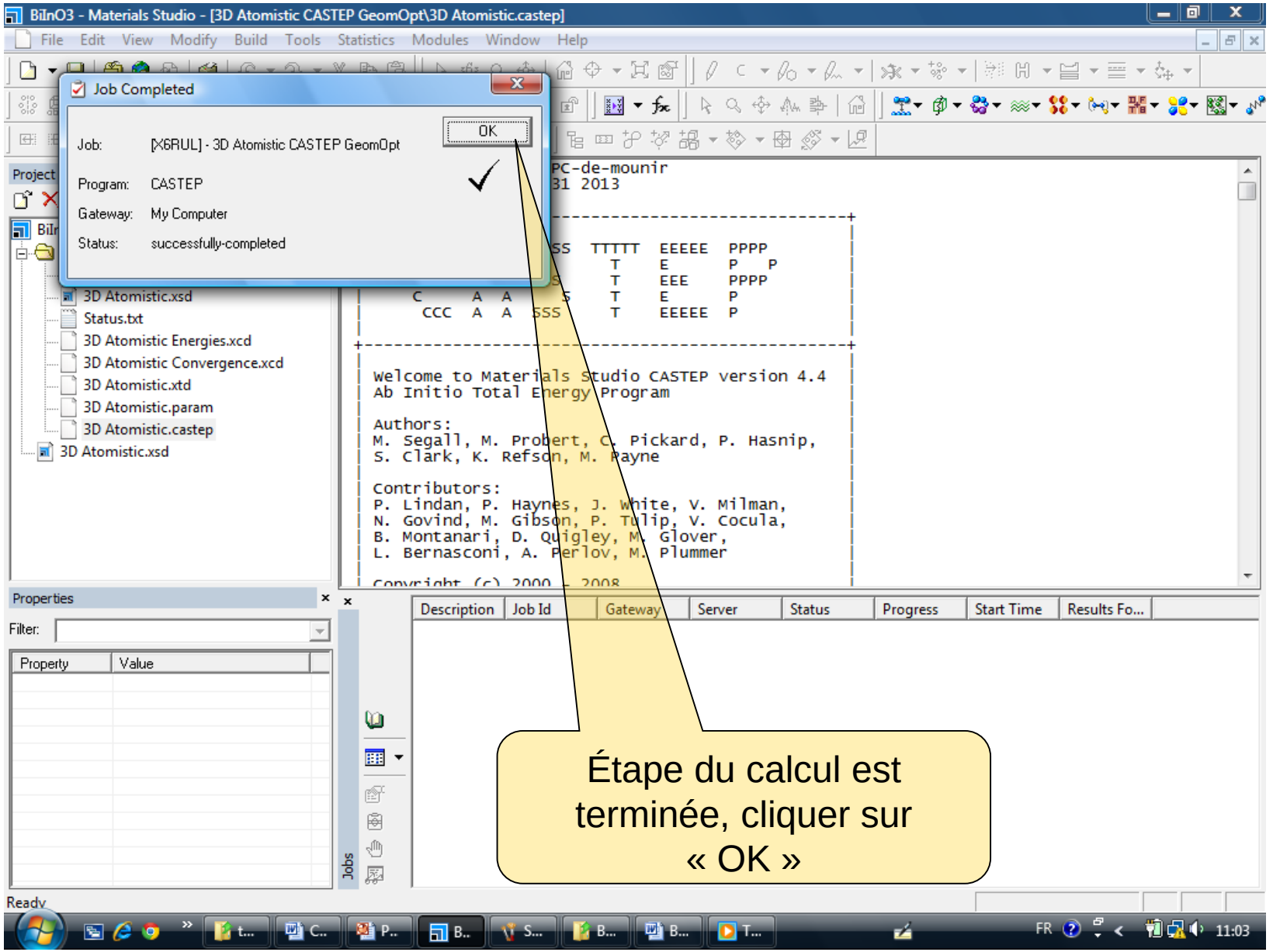

BiInO3 - Materials Studio - [3D Atomistic.xsd *]
File Edit View Modify Build Tools Statistics Modules Window Help
Project
CASTEP Electronic Options
Basis SCF k-points Potentials
Gamma point only
Quality: Fine
Separation: 0,05 1/Å
Custom grid parameters
Monkhorst-Pack grid
a b c
Grid parameters: 6 6 6
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
Description
Ready

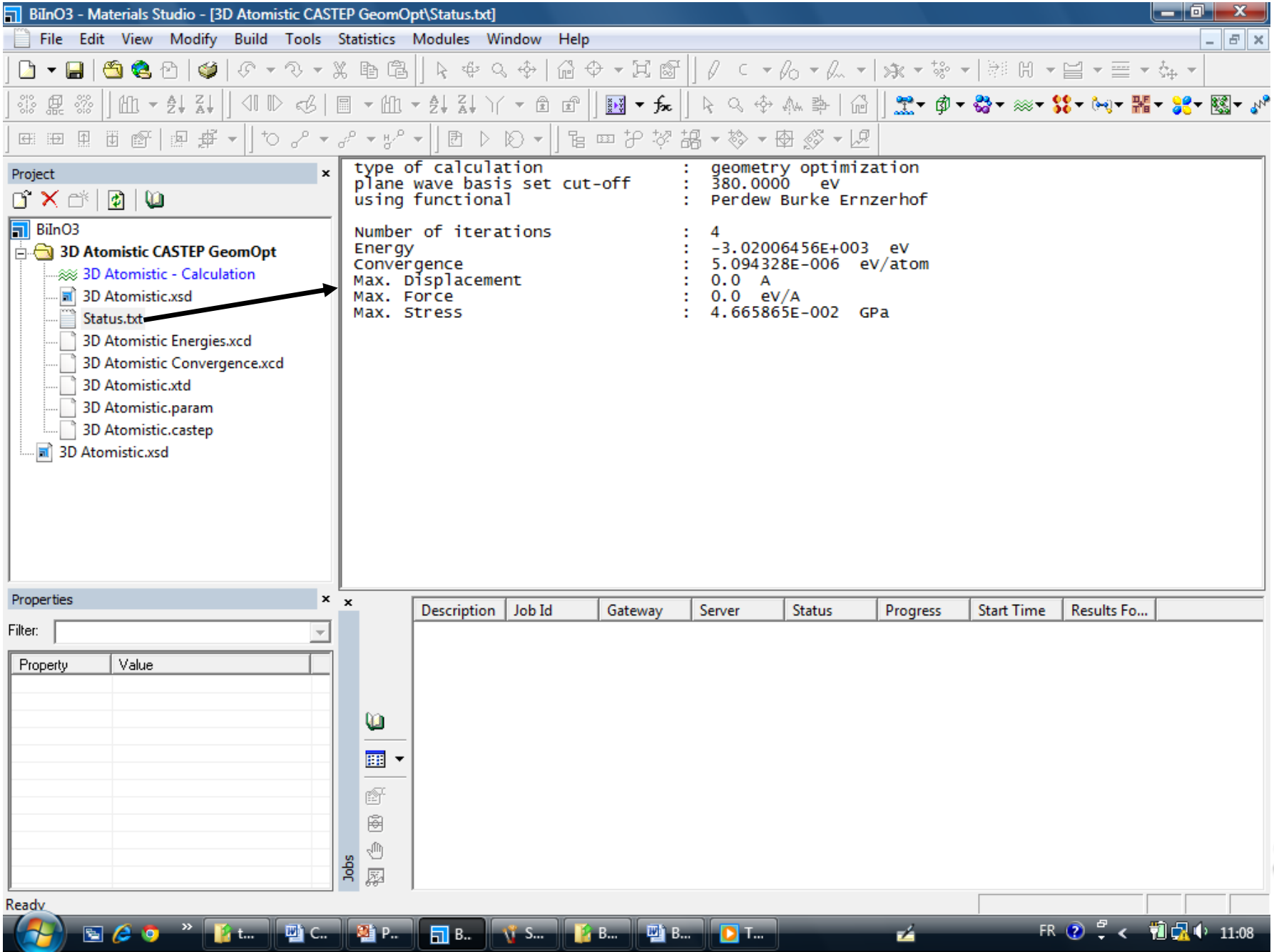
Appuyer sur « Run » pour demarer la procédure du calcul
.

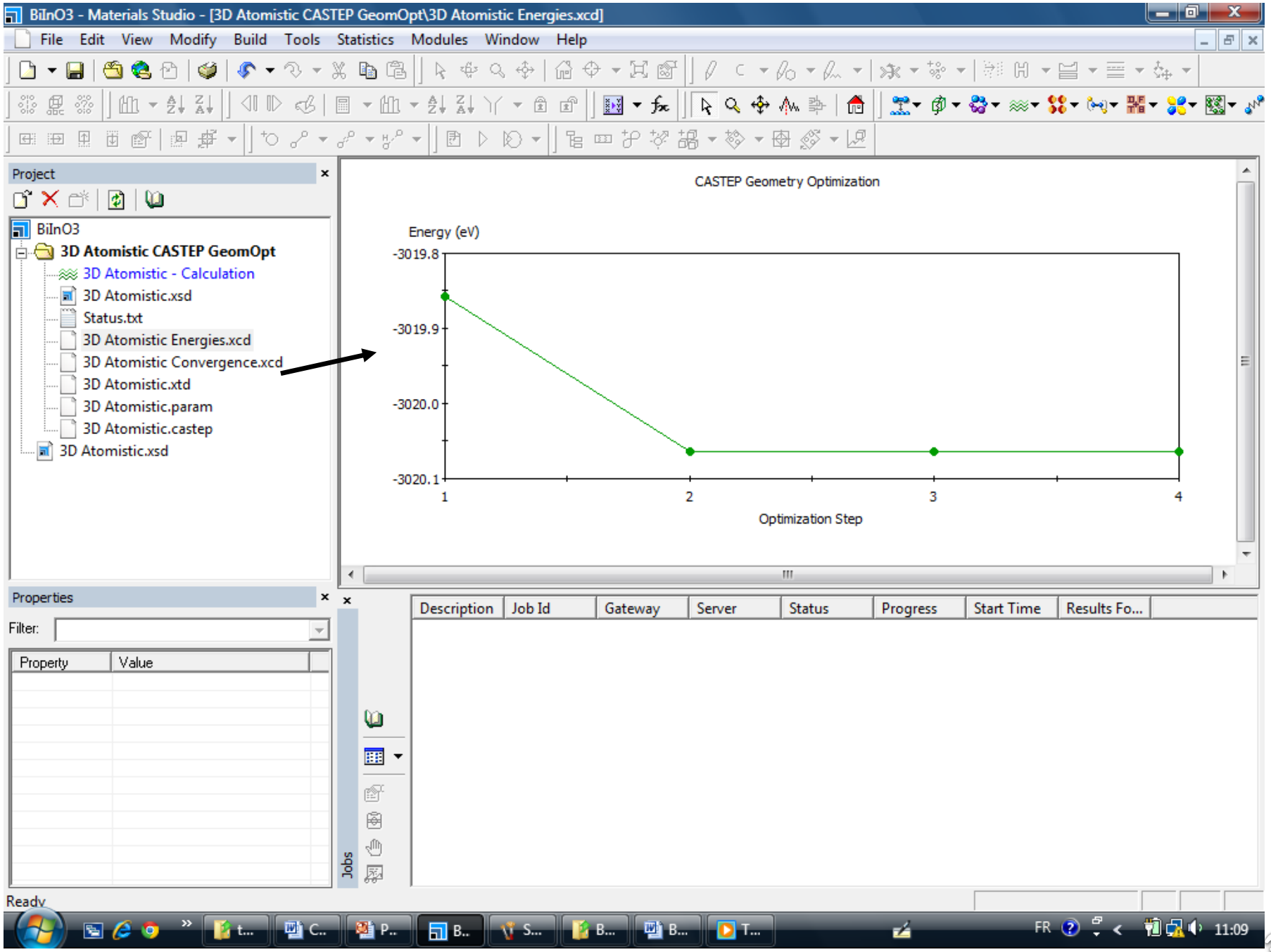
Faire associer tous les processeurs de votre machine pour accélérer le calcul.

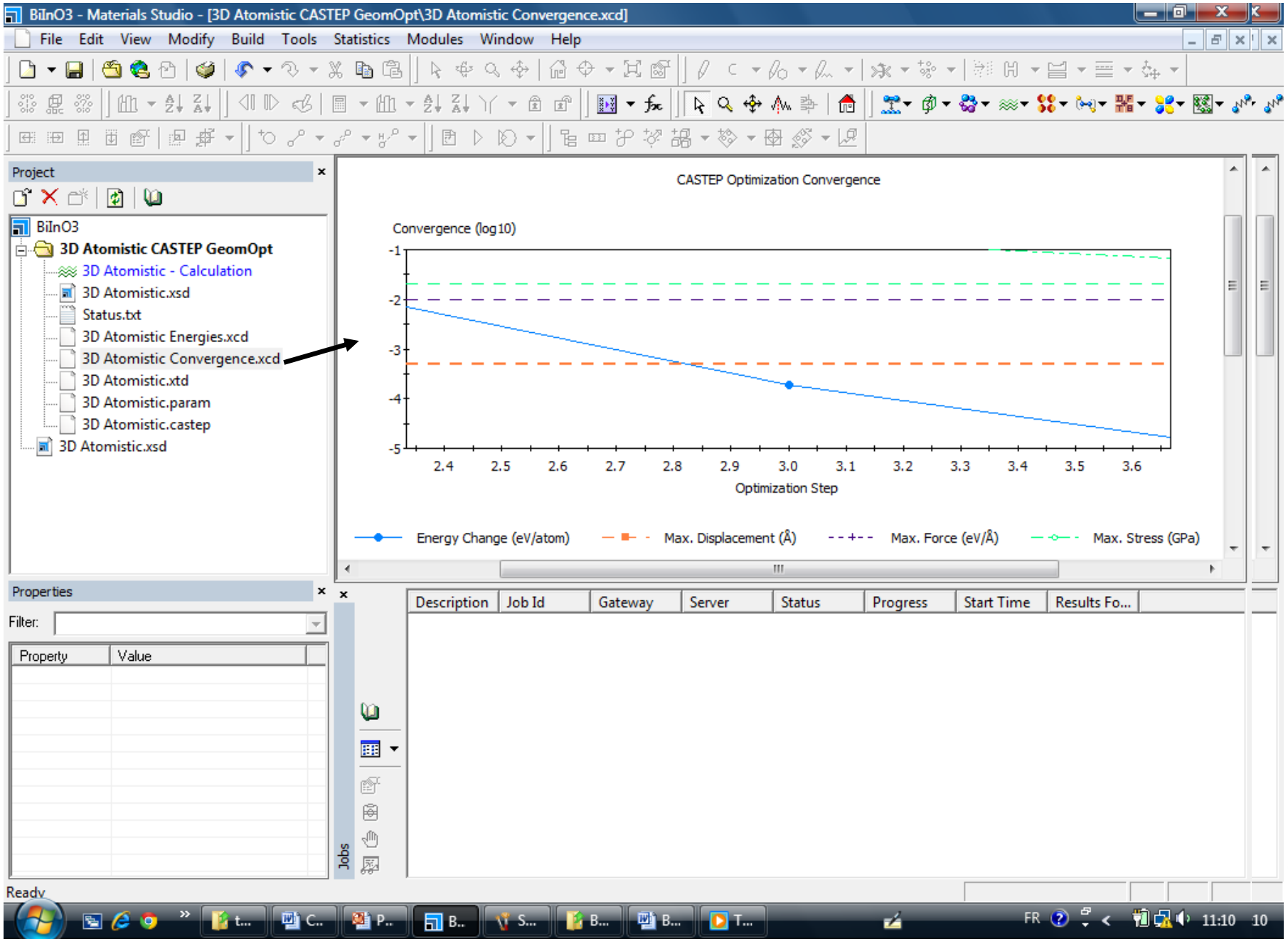


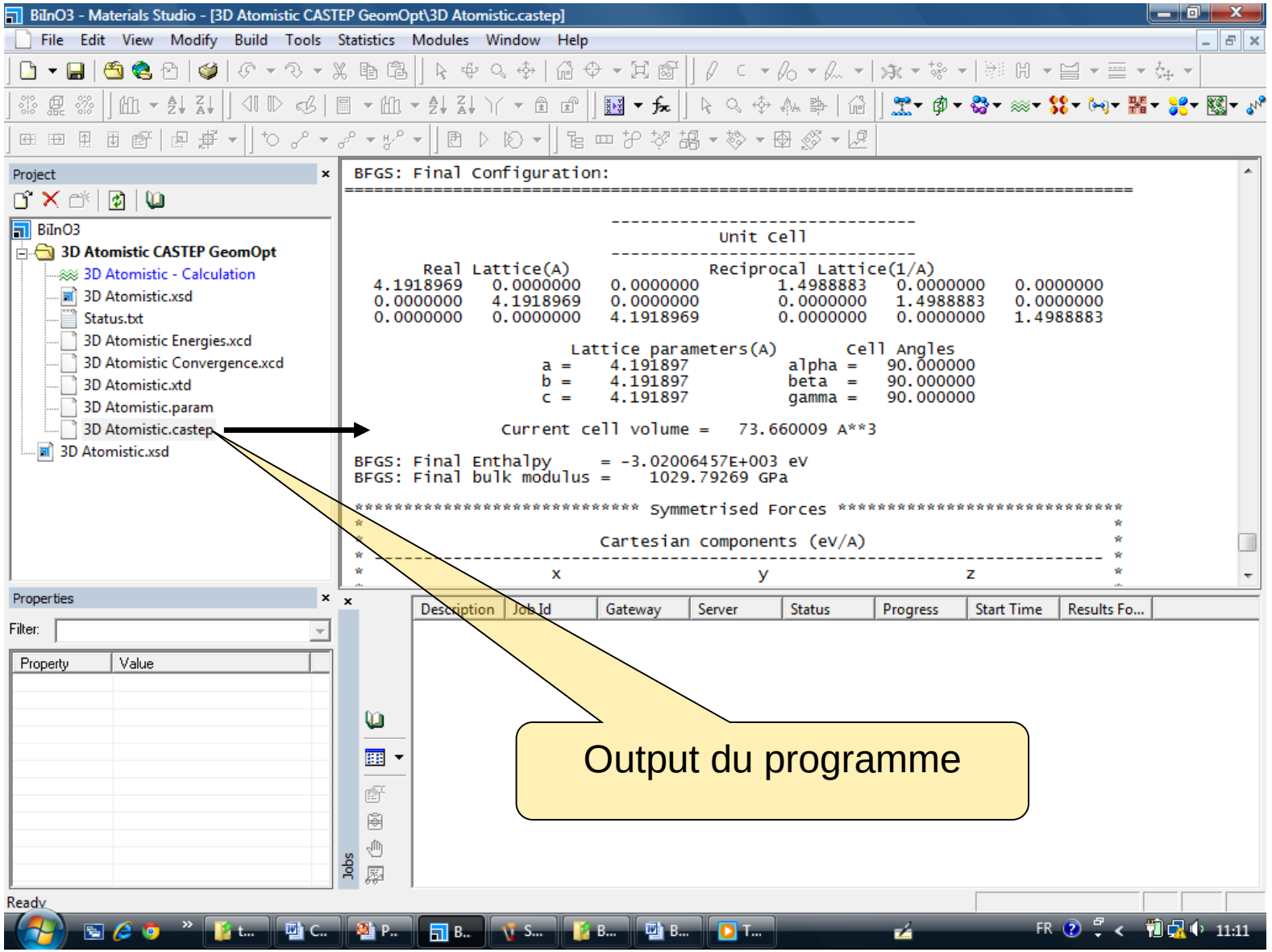

BiInO3 - Materials Studio - [3D Atomistic.xsd *]
File Edit View Modify Build Tools Statistics Modules Window Help
Project
BiInO3
3D Atomistic CASTEP GeomOpt
3D Atomistic - Calculation
3D Atomistic.xsd
3D Atomistic.xsd
Properties
Filter: All
Property Value
Name
Style
Jobs
Description Job Id Gateway Server Status Progress Start Time Results Fo...
3D Ato... X6RUL localhost:... CASTEP running 02/04/201... .\3D Ato...
Le programme en état de calcul
Ready
FR 10:56

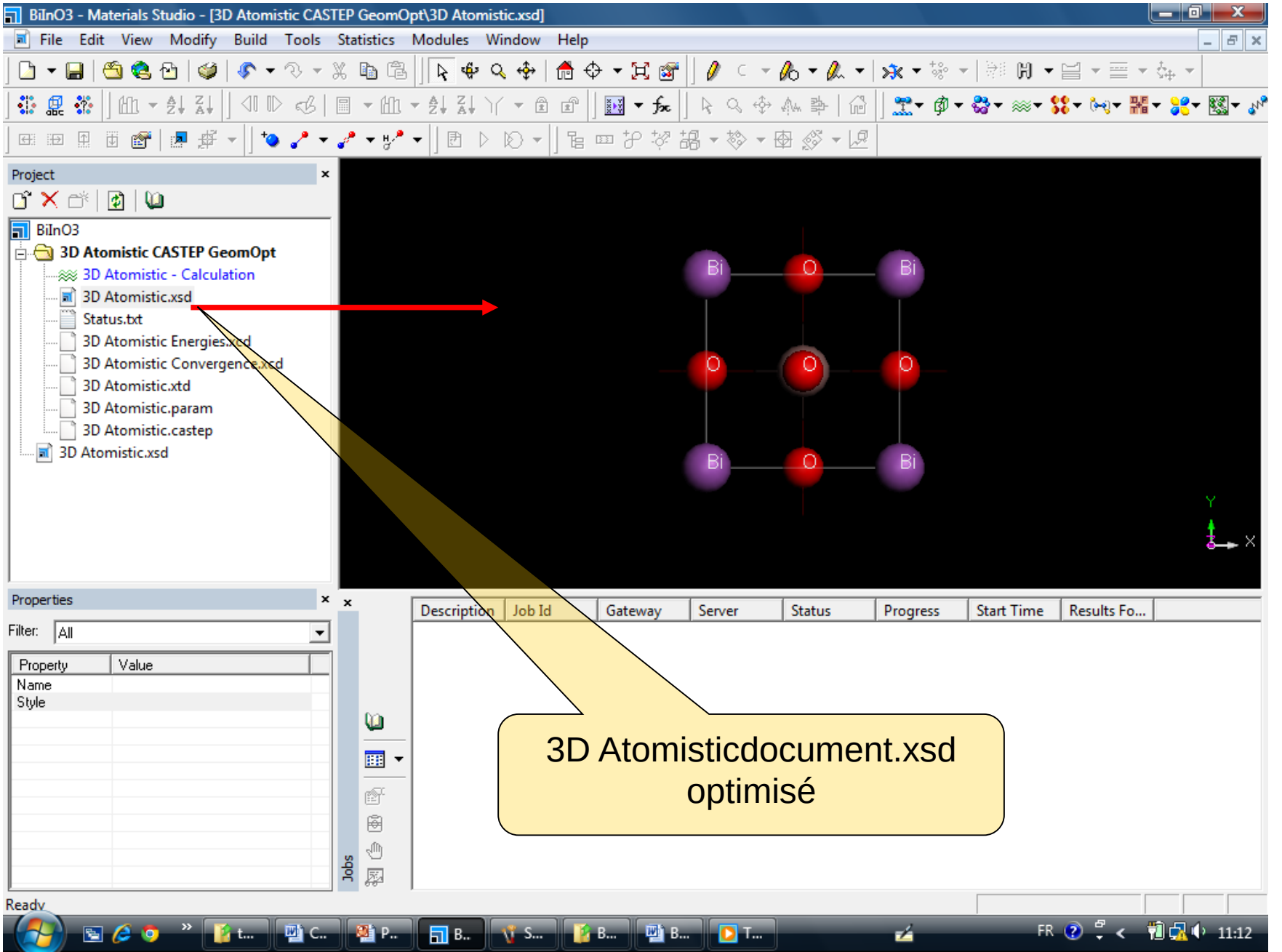

BiInO3 - Materials Studio - [3D Atomistic CASTEP GeomOpt\3D Atomistic.castep]
File Edit View Modify Build Tools Statistics Modules Window Help
Job Completed
Job: [X6RUL] - 3D Atomistic CASTEP GeomOpt
Program: CASTEP
Gateway: My Computer
Status: successfully-completed
OK
Project
3D Atomistic.xsd
Status.txt
3D Atomistic Energies.xcd
3D Atomistic Convergence.xcd
3D Atomistic.xtd
3D Atomistic.param
3D Atomistic.castep
3D Atomistic.xsd
PC-de-mounir
31 2013
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
Properties
Filter:
Property
Value
Description
Job Id
Gateway
Server
Status
Progress
Start Time
Results Fo...
Jobs
Ready
Étape du calcul est terminée, cliquer sur « OK »


BiInO3 - Materials Studio - [3D Atomistic CASTEP GeomOpt\Status.txt]
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
type of calculation : geometry optimization
plane wave basis set cut-off : 380.0000 eV
using functional : Perdew Burke Ernzerhof
Number of iterations : 4
Energy : -3.02006456E+003 eV
Convergence : 5.094328E-006 eV/atom
Max. Displacement : 0.0 A
Max. Force : 0.0 eV/A
Max. Stress : 4.665865E-002 GPa
Properties
Filter:
Property
Value
Jobs
Description
Job Id
Gateway
Server
Status
Progress
Start Time
Results Fo...
Ready
FR
11:08


BiInO3 - Materials Studio - [3D Atomistic CASTEP GeomOpt\3D Atomistic Energies.xcd]
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 Geometry Optimization
Energy (eV)
-3019.8
-3019.9
-3020.0
-3020.1
1
2
3
4
Optimization Step
Properties
Filter:
Property
Value
Description
Job Id
Gateway
Server
Status
Progress
Start Time
Results Fo...
Jobs
Ready
FR
11:09

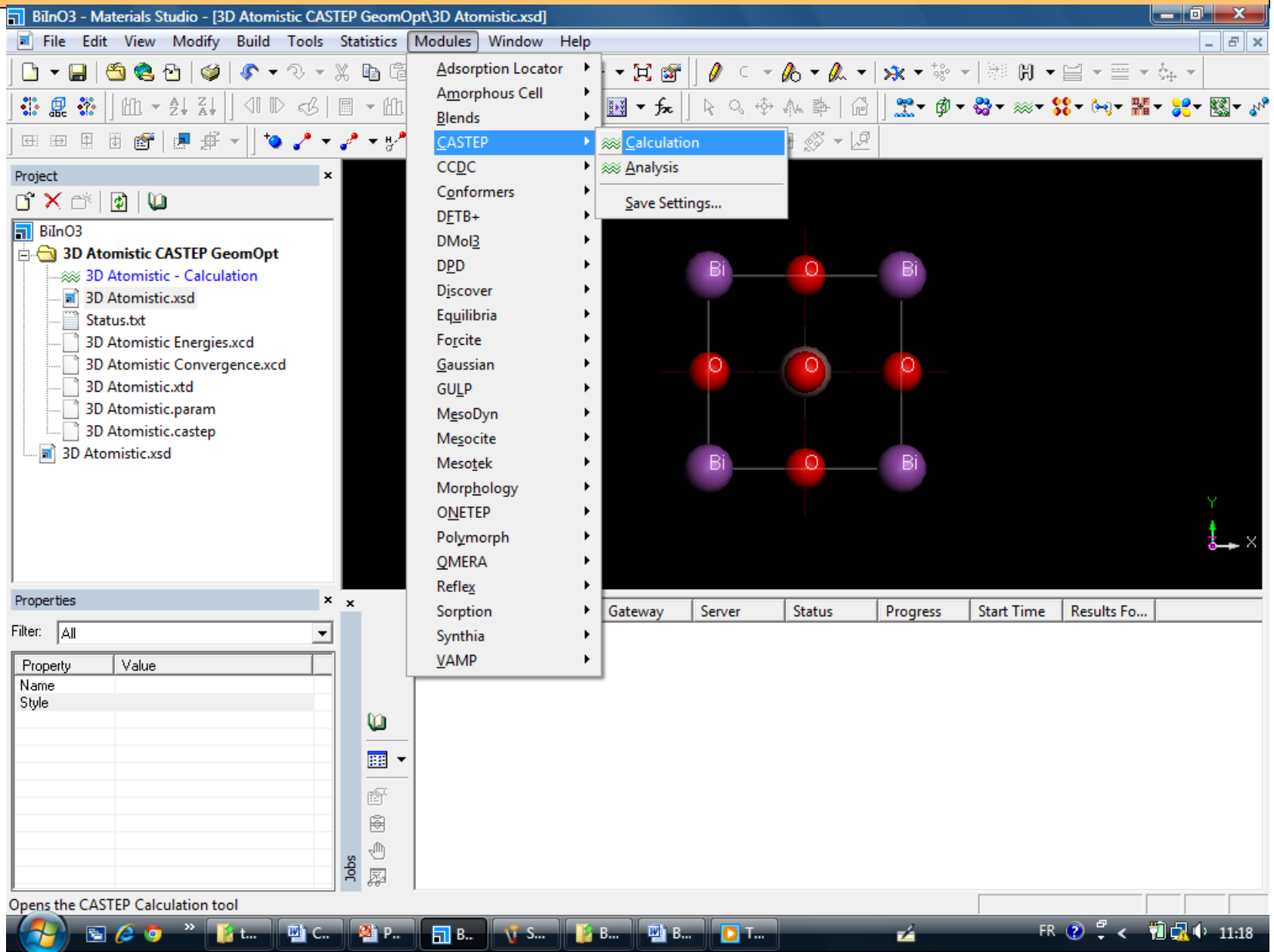

BiInO3 - Materials Studio - [3D Atomistic CASTEP GeomOpt\3D Atomistic Convergence.xcd]
File Edit View Modify Build Tools Statistics Modules Window Help
Project
BiInO3
3D Atomistic CASTEP GeomOpt
3D Atomistic - Calculation
3D Atomistic.xsd
Status.txt
3D Atomistic Energies.xcd
3D Atomistic Convergence.xcd
3D Atomistic.xtd
3D Atomistic.param
3D Atomistic.castep
3D Atomistic.xsd
CASTEP Optimization Convergence
Convergence (log10)
-1
-2
-3
-4
-5
2.4 2.5 2.6 2.7 2.8 2.9 3.0 3.1 3.2 3.3 3.4 3.5 3.6
Optimization Step
Energy Change (eV/atom)
Max. Displacement (Å)
Max. Force (eV/Å)
Max. Stress (GPa)
Properties
Filter:
Property
Value
Description
Job Id
Gateway
Server
Status
Progress
Start Time
Results Fo...
Jobs
Ready
11:10


BiInO3 - Materials Studio - [3D Atomistic CASTEP GeomOpt\3D Atomistic.castep]
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
BFGS: Final Configuration:
Unit Cell
Real Lattice(A)
Reciprocal Lattice(1/A)
4.1918969 0.0000000 0.0000000 1.4988883 0.0000000 0.0000000
0.0000000 4.1918969 0.0000000 0.0000000 1.4988883 0.0000000
0.0000000 0.0000000 4.1918969 0.0000000 0.0000000 1.4988883
Lattice parameters(A) Cell Angles
a = 4.191897 alpha = 90.000000
b = 4.191897 beta = 90.000000
c = 4.191897 gamma = 90.000000
Current cell volume = 73.660009 A**3
BFGS: Final Enthalpy = -3.02006457E+003 eV
BFGS: Final bulk modulus = 1029.79269 GPa
Symmetrised Forces
Cartesian components (eV/A)
x y z
Properties
Filter:
Property Value
Description Job Id Gateway Server Status Progress Start Time Results Fo...
Jobs
Ready
Output du programme

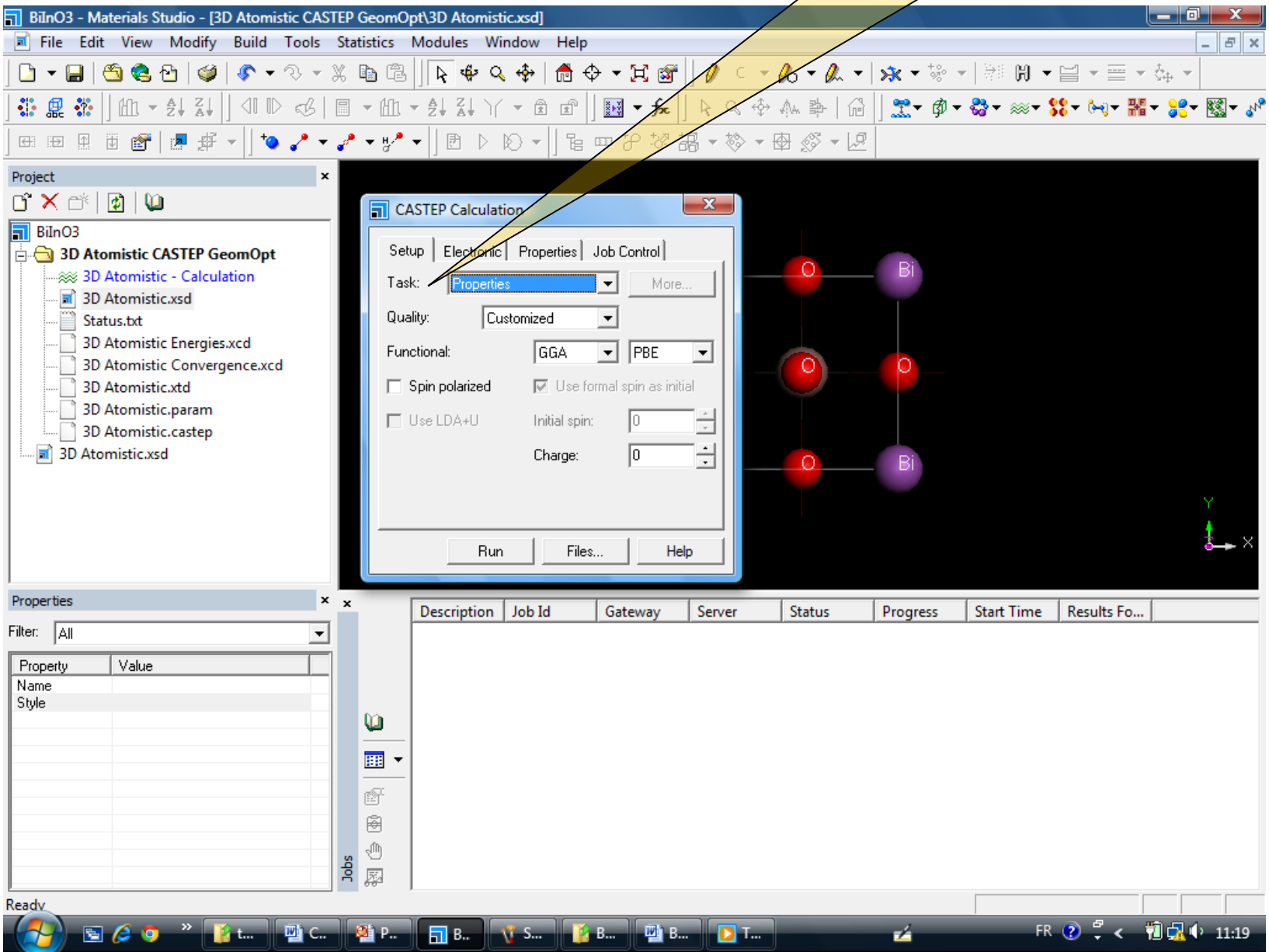

BiInO3 - Materials Studio - [3D Atomistic CASTEP GeomOpt\3D Atomistic.xsd]
File Edit View Modify Build Tools Statistics Modules Window Help
Project
BiInO3
3D Atomistic CASTEP GeomOpt
3D Atomistic - Calculation
3D Atomistic.xsd
Status.txt
3D Atomistic Energies.xsd
3D Atomistic Convergence.xsd
3D Atomistic.xtd
3D Atomistic.param
3D Atomistic.castep
3D Atomistic.xsd
Bi O Bi
O O O
Bi O Bi
Y
X
Properties
Filter: All
Property Value
Name
Style
Description Job Id Gateway Server Status Progress Start Time Results Fo...
Jobs
3D Atomisticdocument.xsd optimisé
Ready
FR 11:12

Calcul des propriétés électronique et optique

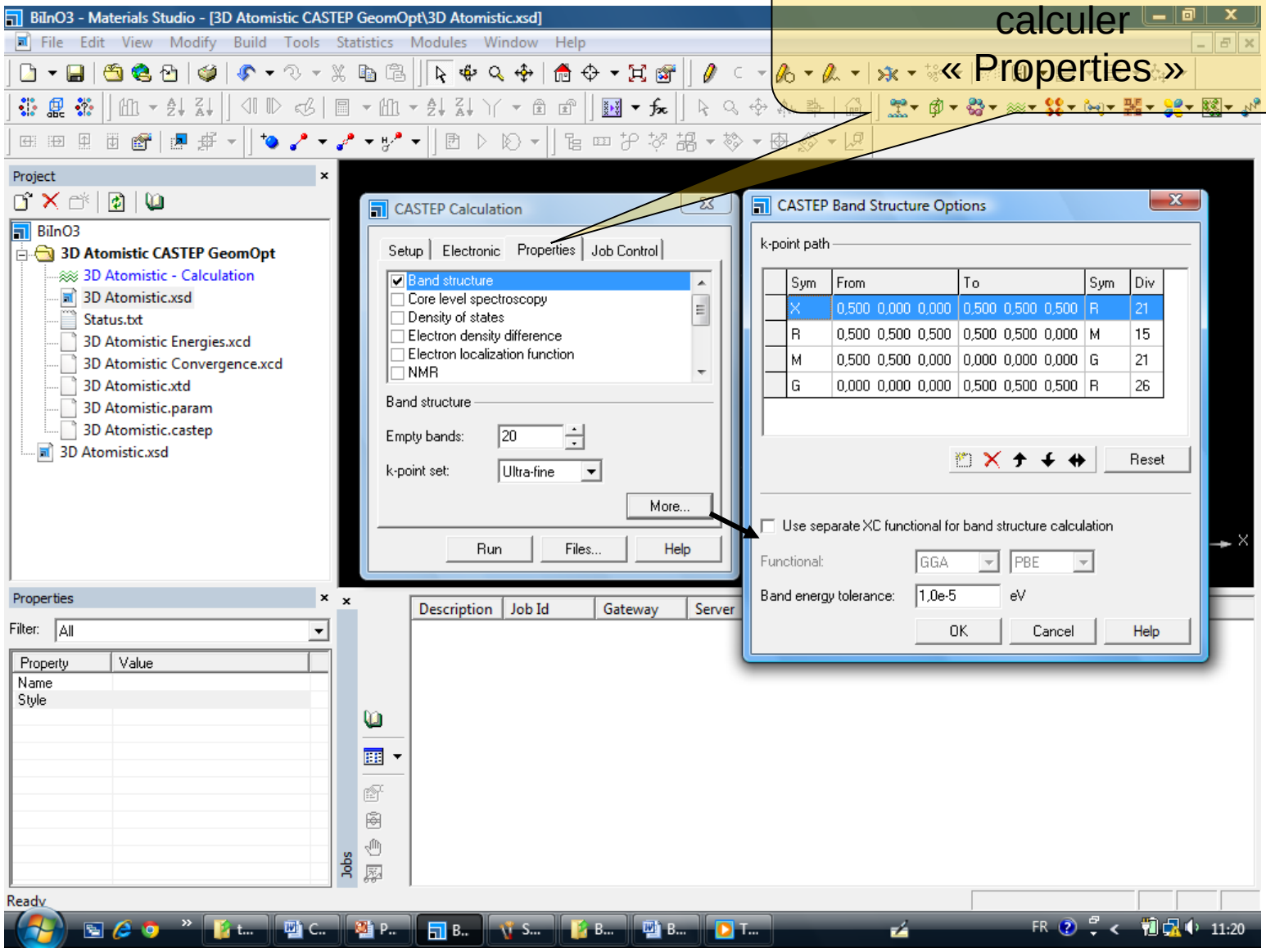
Une fois que le calcul d'optimisation géométrique est termine, on lance notre calcul des propretés à partir du fichier « 3D Atomistic Document.xsd »

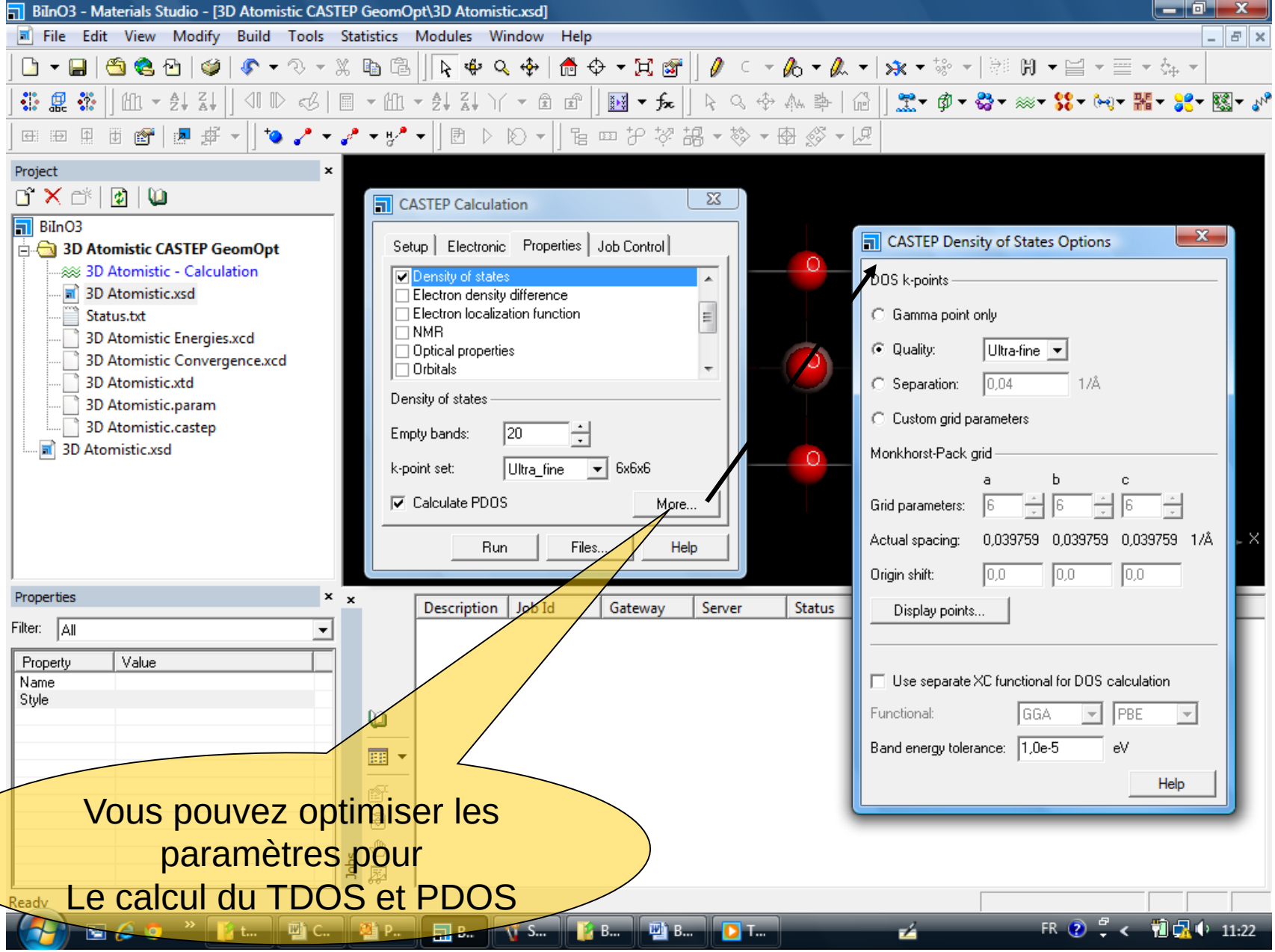


Tache est active sur
« Properties »

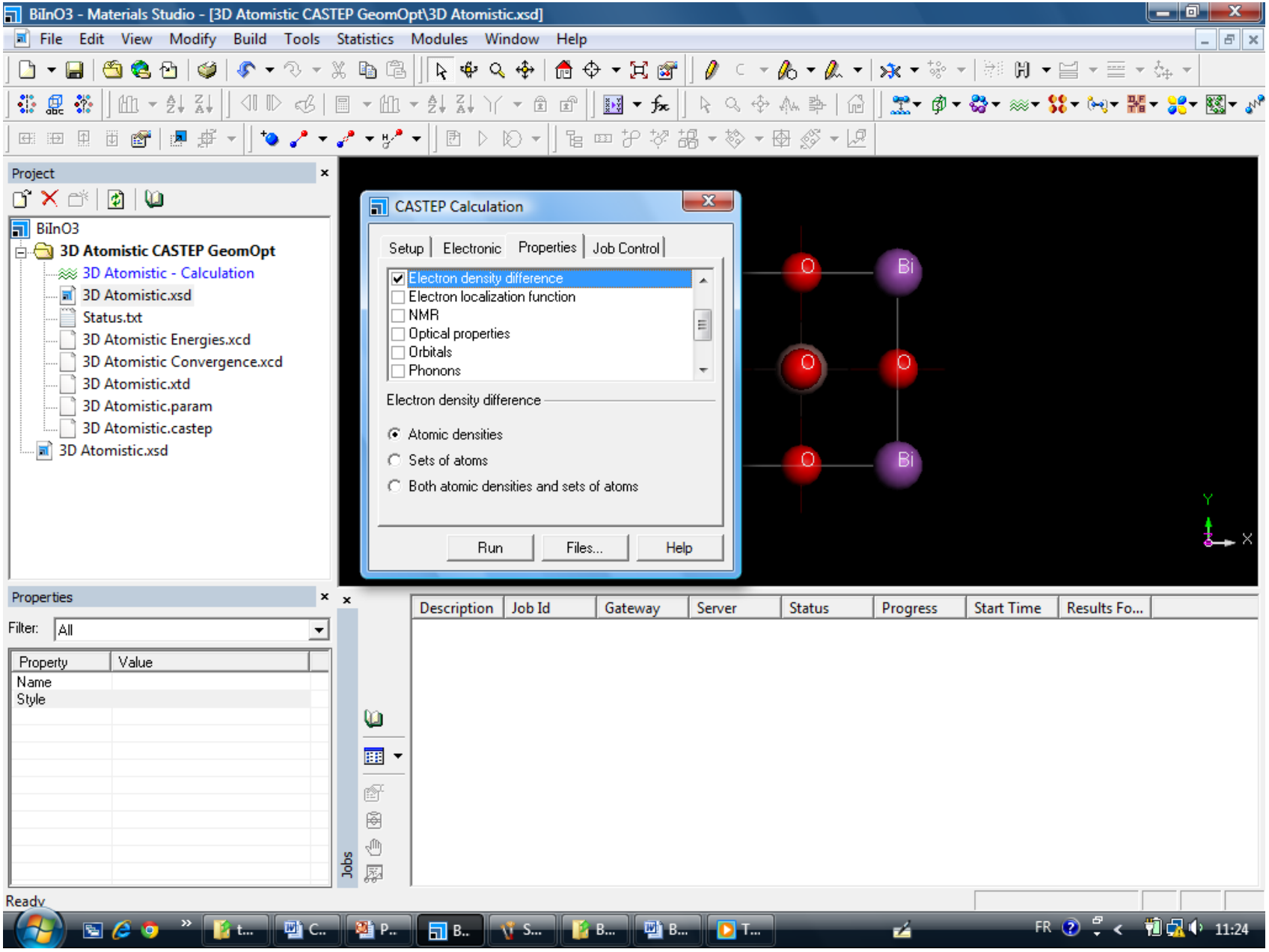


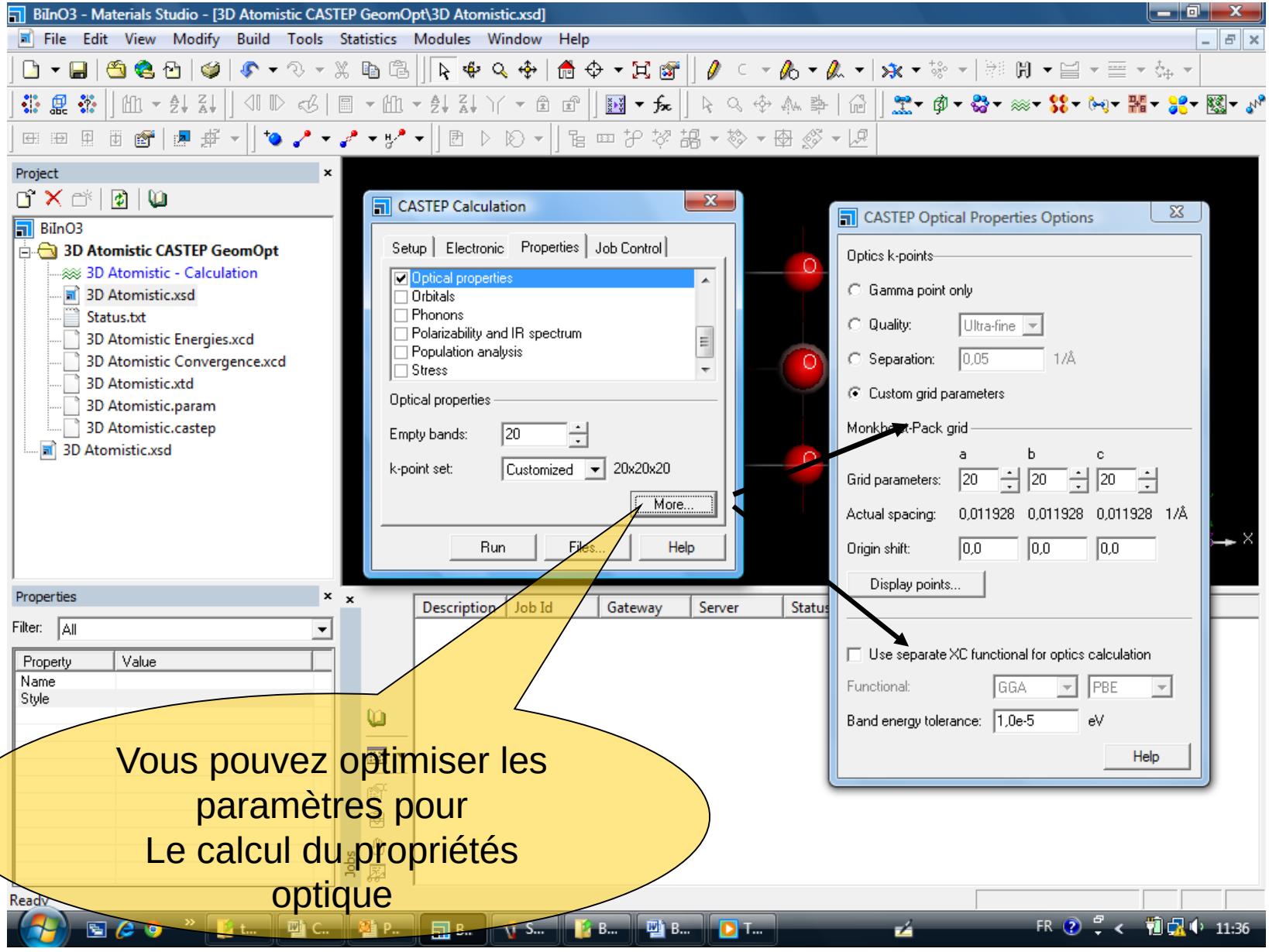
Coucher les propriétés à calculer « Properties »



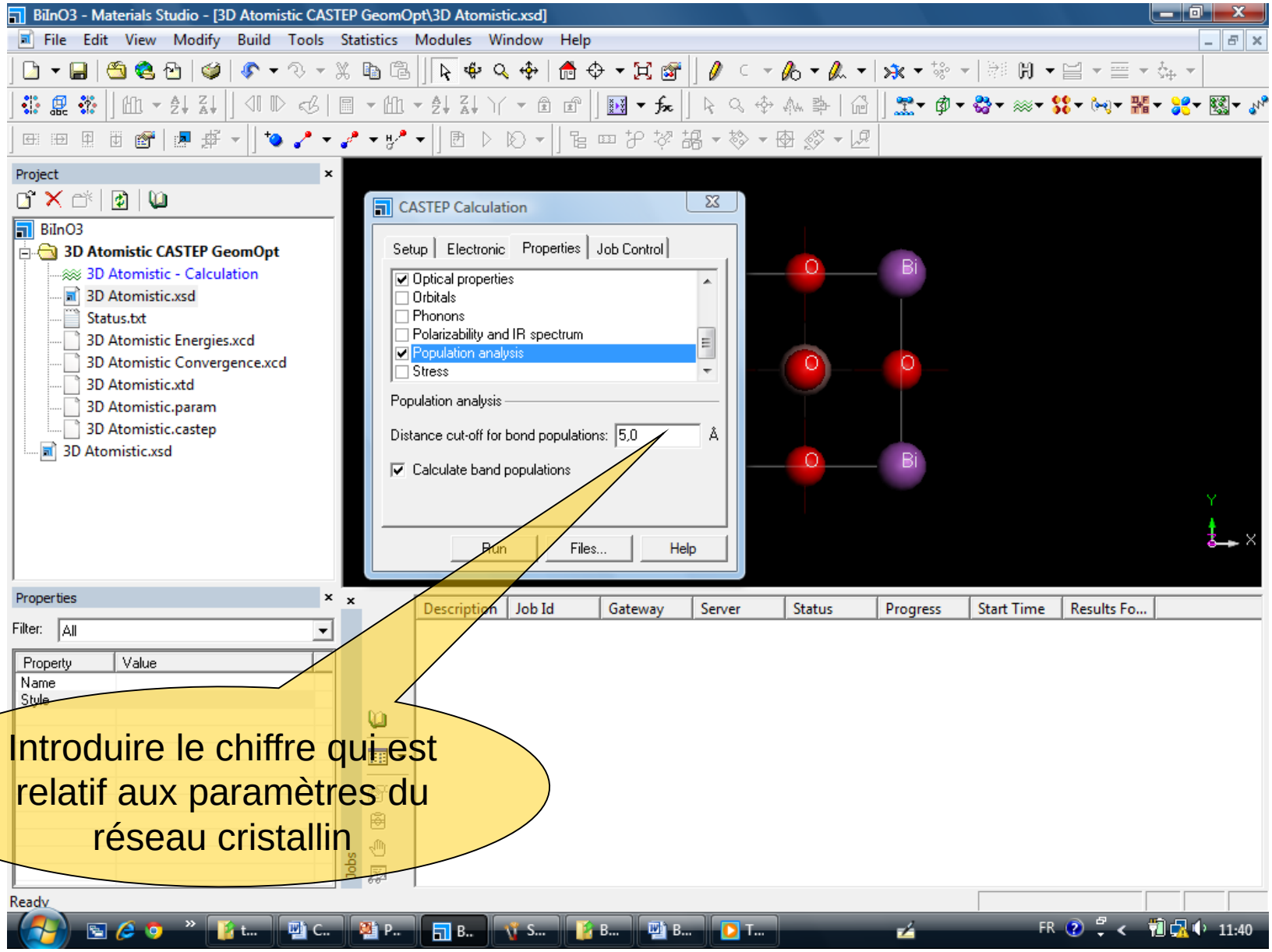


Vous pouvez optimiser les paramètres pour
Le calcul du TDOS et PDOS

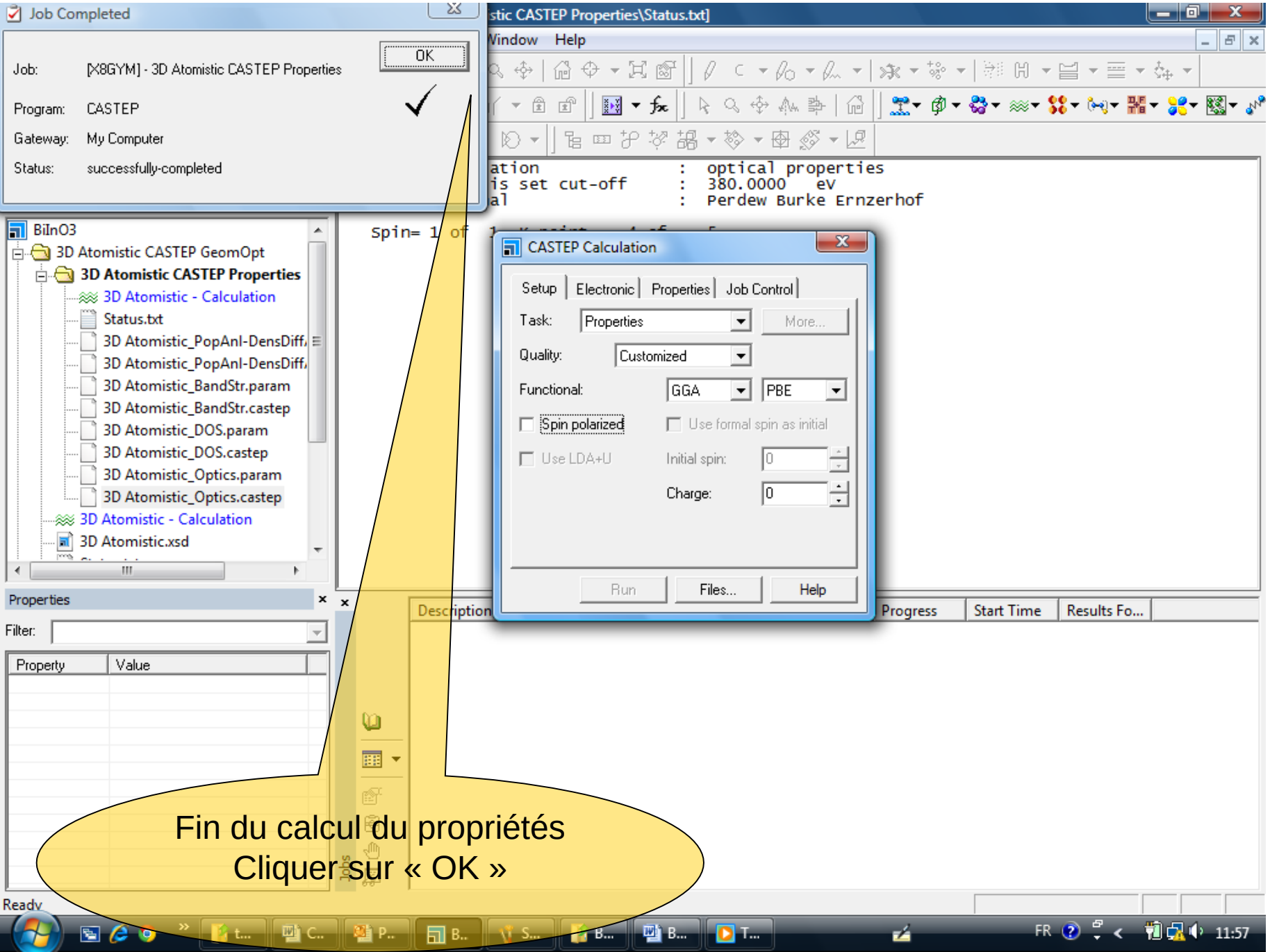

BiInO3 - Materials Studio - [3D Atomistic CASTEP GeomOpt\3D Atomistic.xsd]
File Edit View Modify Build Tools Statistics Modules Window Help
Project
BiInO3
3D Atomistic CASTEP GeomOpt
3D Atomistic - Calculation
3D Atomistic.xsd
Status.txt
3D Atomistic Energies.xcd
3D Atomistic Convergence.xcd
3D Atomistic.xtd
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
O
Bi
Properties
Filter: All
Property Value
Name
Style
Description Job Id Gateway Server Status Progress Start Time Results Fo...
Jobs
Ready
11:24



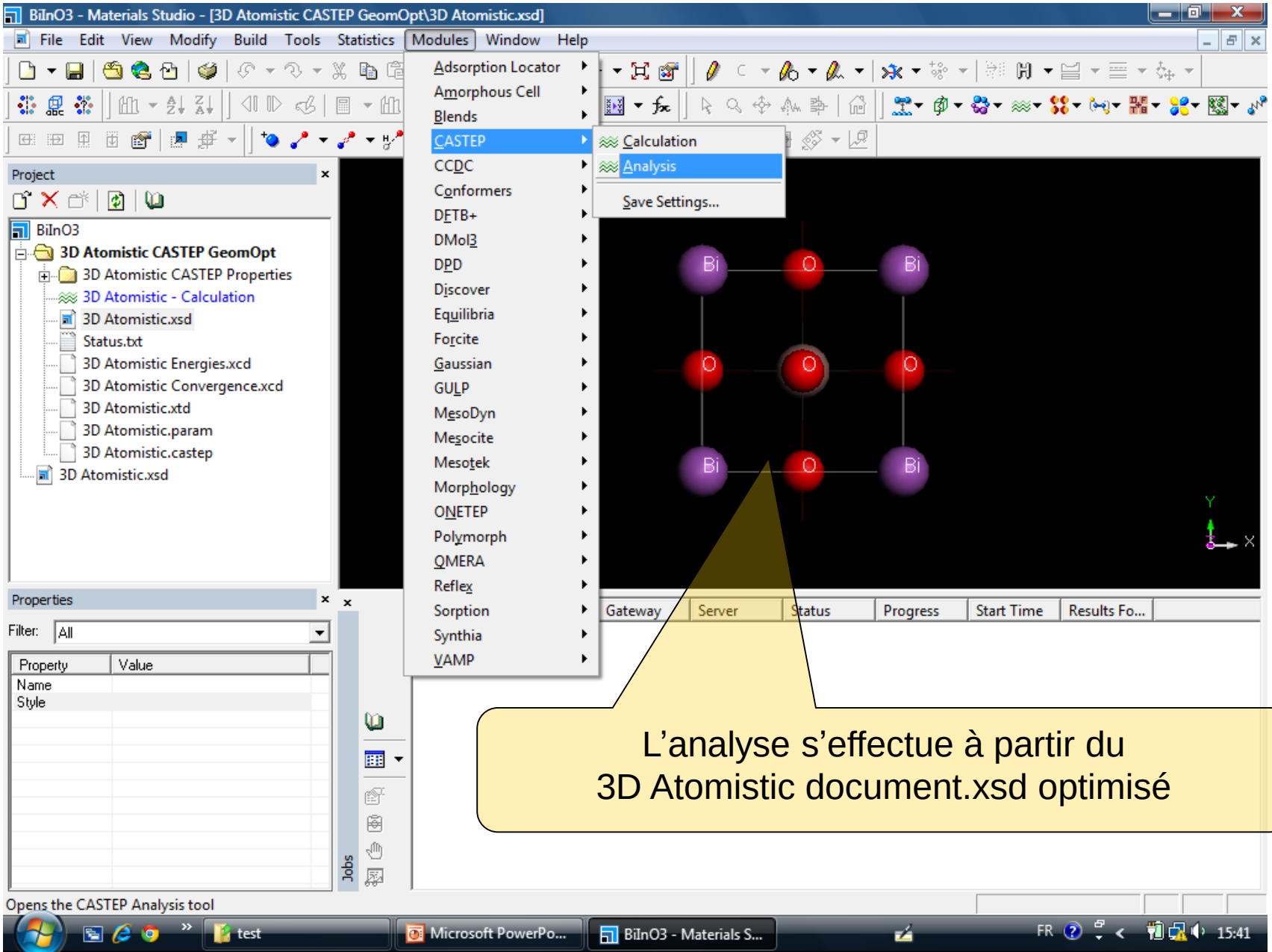
Vous pouvez optimiser les paramètres pour Le calcul du propriétés optique



Introduire le chiffre qui est relatif aux paramètres du réseau cristallin

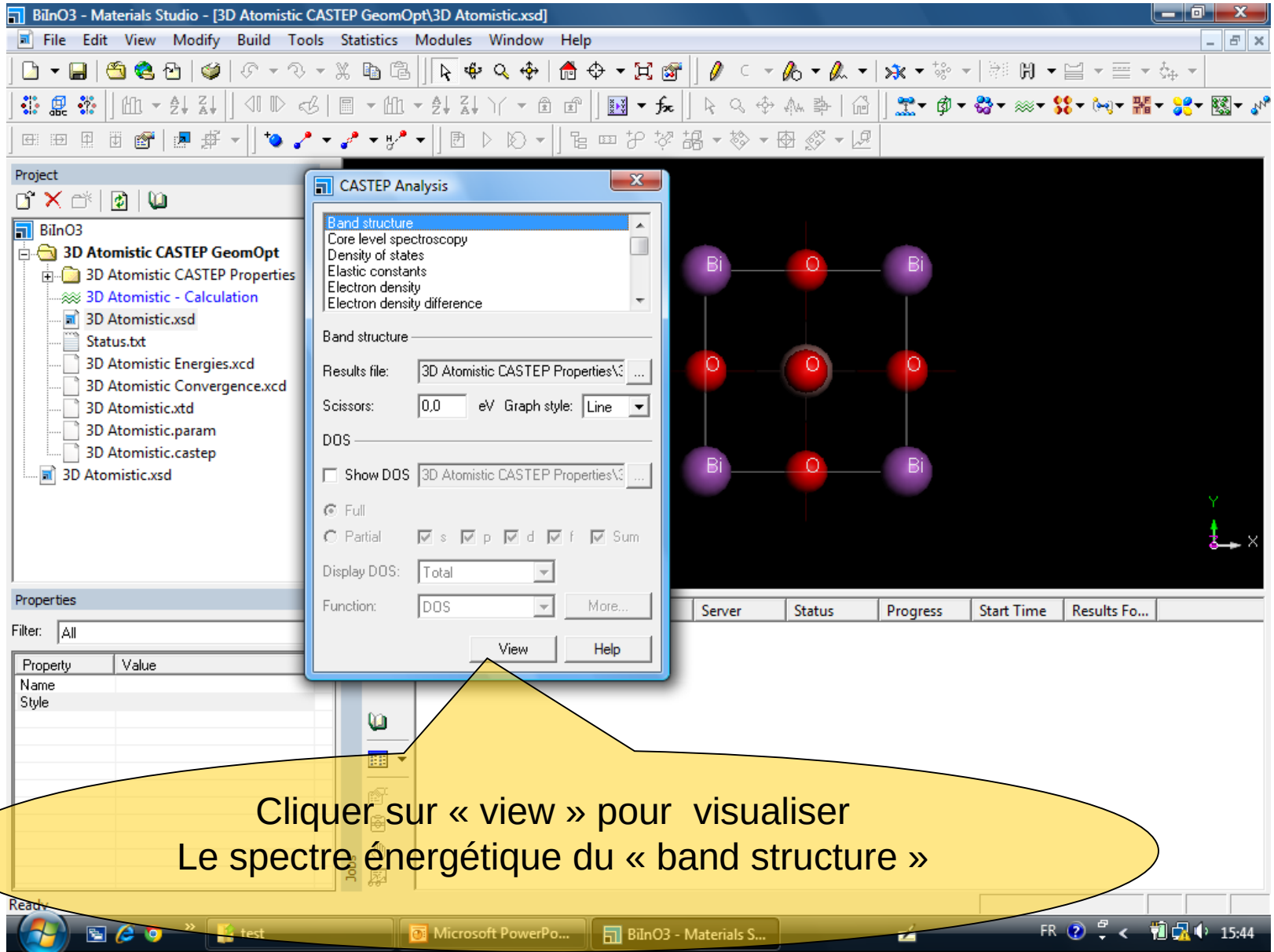

Job Completed
Job: [X8GYM] - 3D Atomistic CASTEP Properties
Program: CASTEP
Gateway: My Computer
Status: successfully-completed
OK
stic CASTEP Properties\Status.txt]
Window Help
ation : optical properties
is set cut-off : 380.0000 eV
al : Perdew Burke Ernzerhof
Spin= 1 of
BiInO3
3D Atomistic CASTEP GeomOpt
3D Atomistic CASTEP Properties
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 - Calculation
3D Atomistic.xsd
CASTEP Calculation
Setup
Electronic
Properties
Job Control
Task: Properties
More...
Quality: Customized
Functional: GGA PBE
Spin polarized
Use formal spin as initial
Use LDA+U
Initial spin: 0
Charge: 0
Run
Files...
Help
Properties
Filter:
Property
Value
Description
Progress
Start Time
Results Fo...
Ready
Fin du calcul du propriétés
Cliquer sur « OK »

Analyse des résultats
Pour les propriétés électroniques et optiques

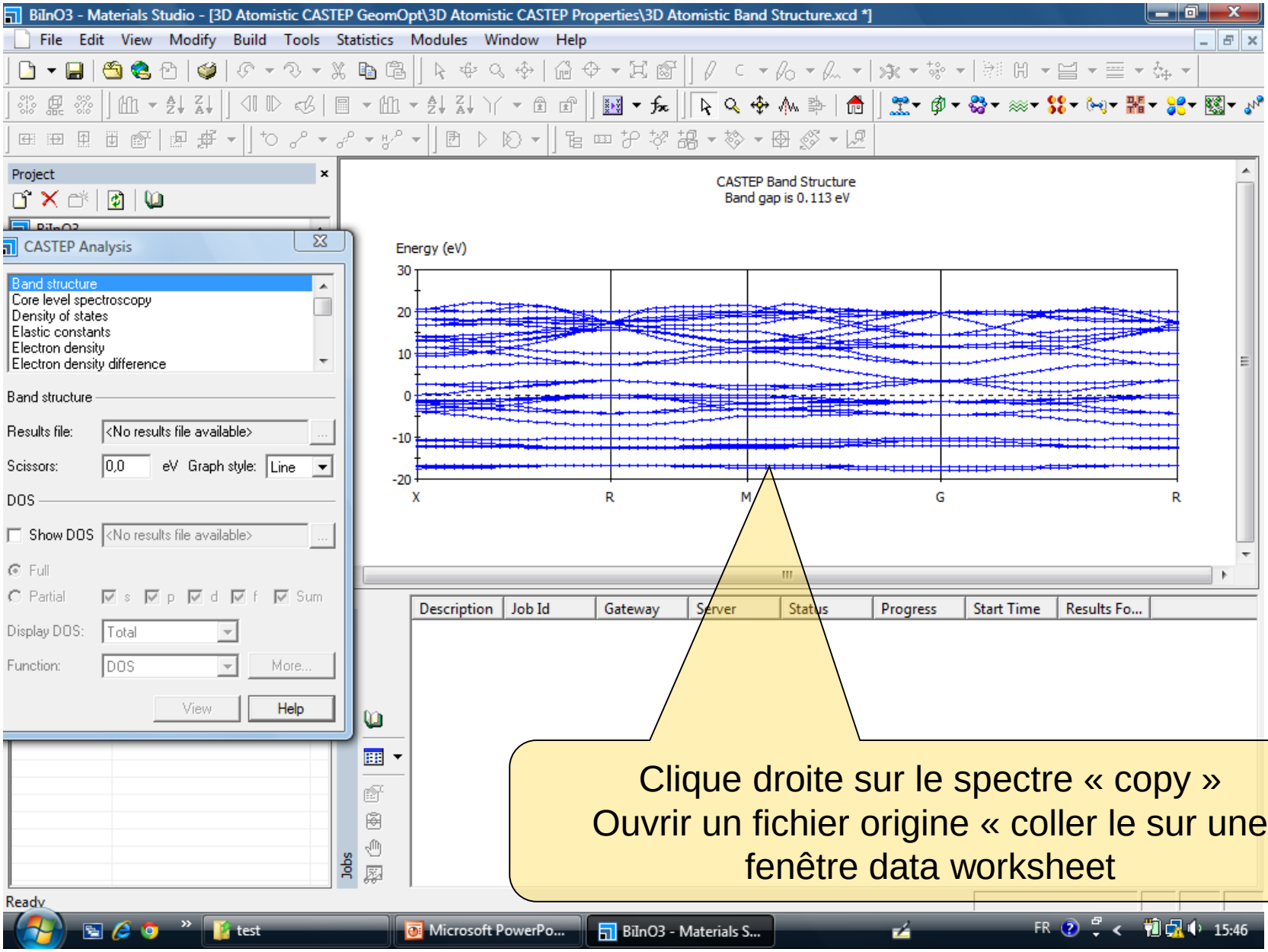


L'analyse s'effectue à partir du 3D Atomistic document.xsd optimisé

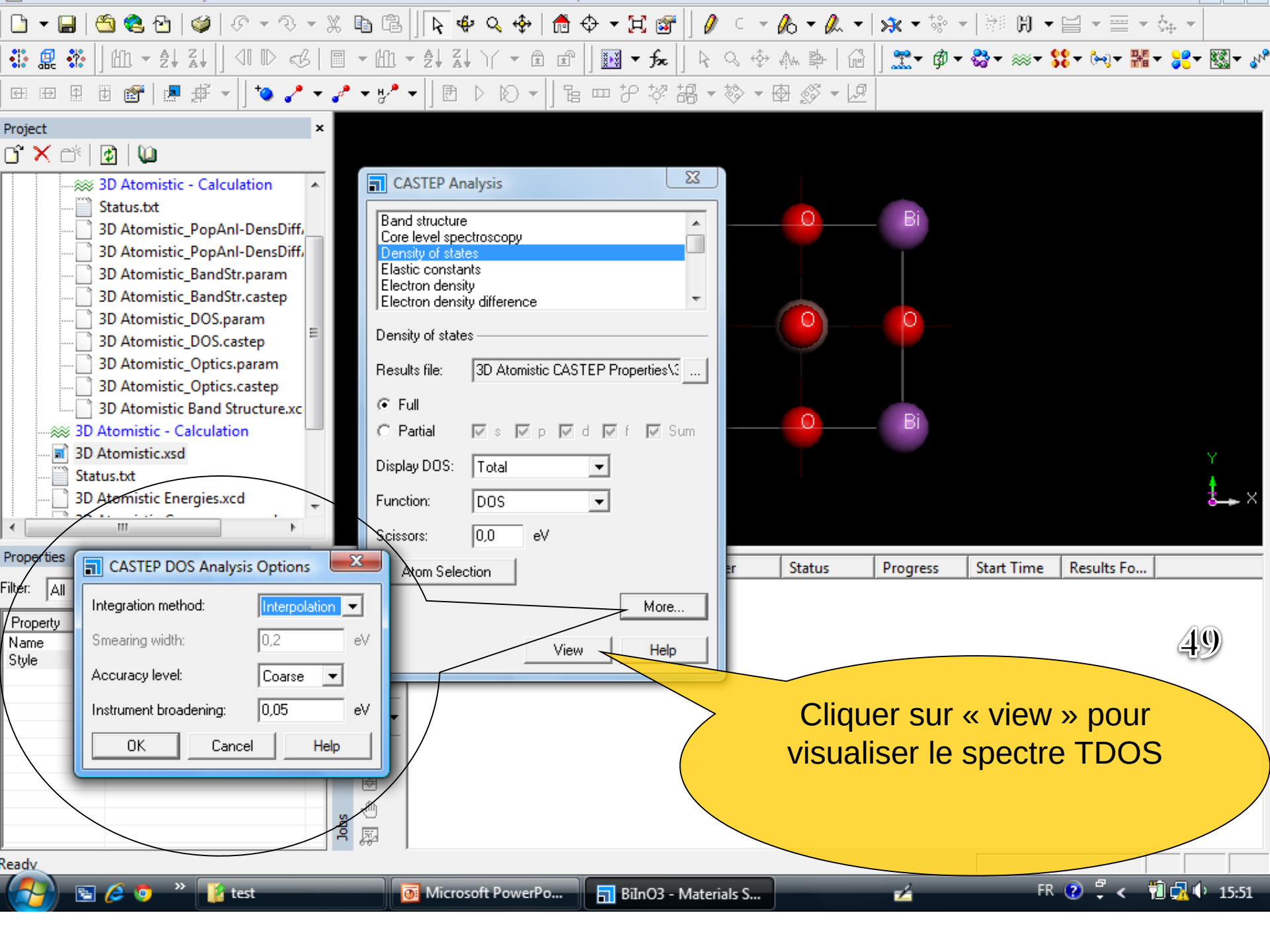
Analyse des Propriétés électronique



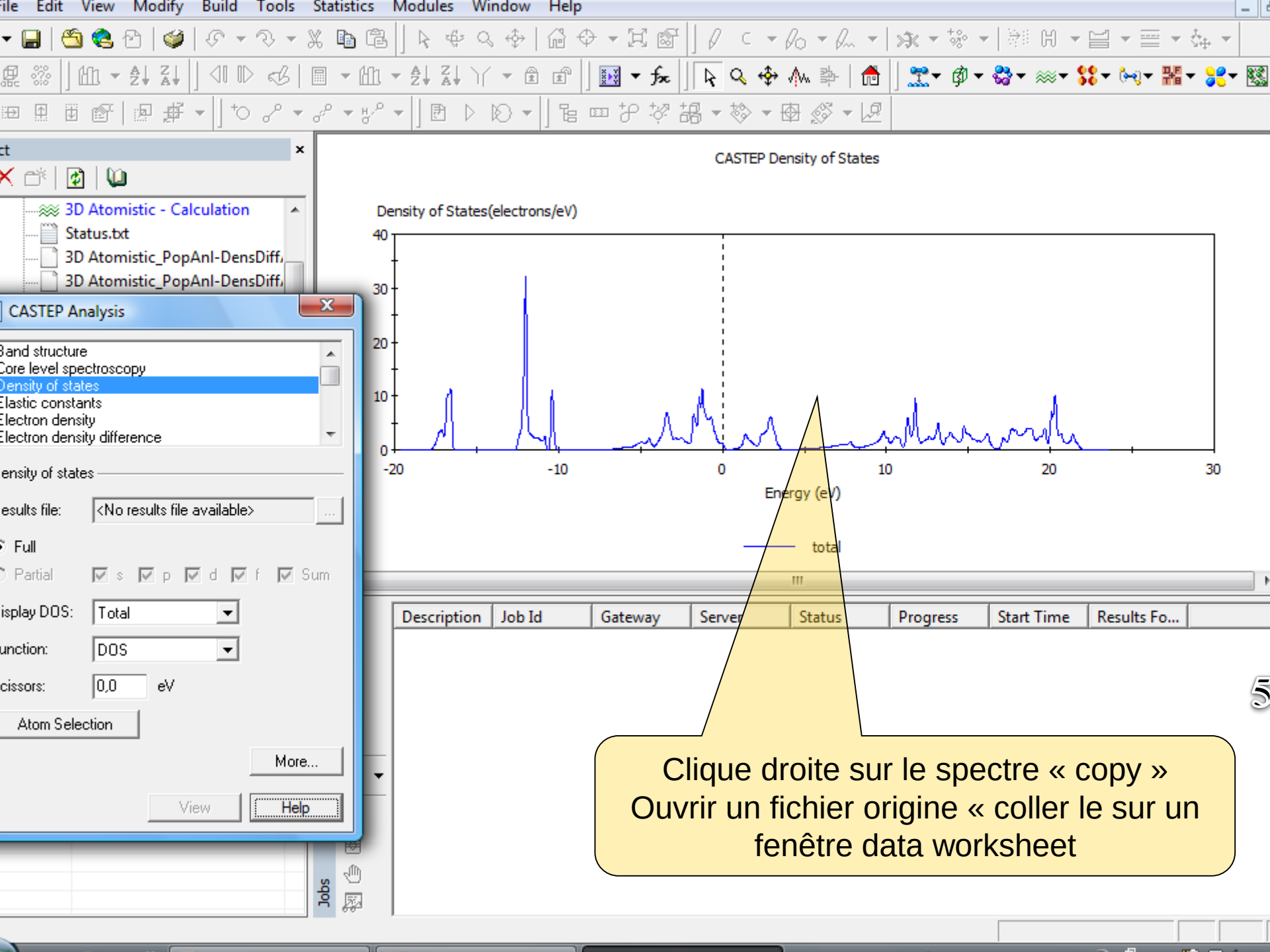
Cliquer sur « view » pour visualiser
Le spectre énergétique du « band structure »

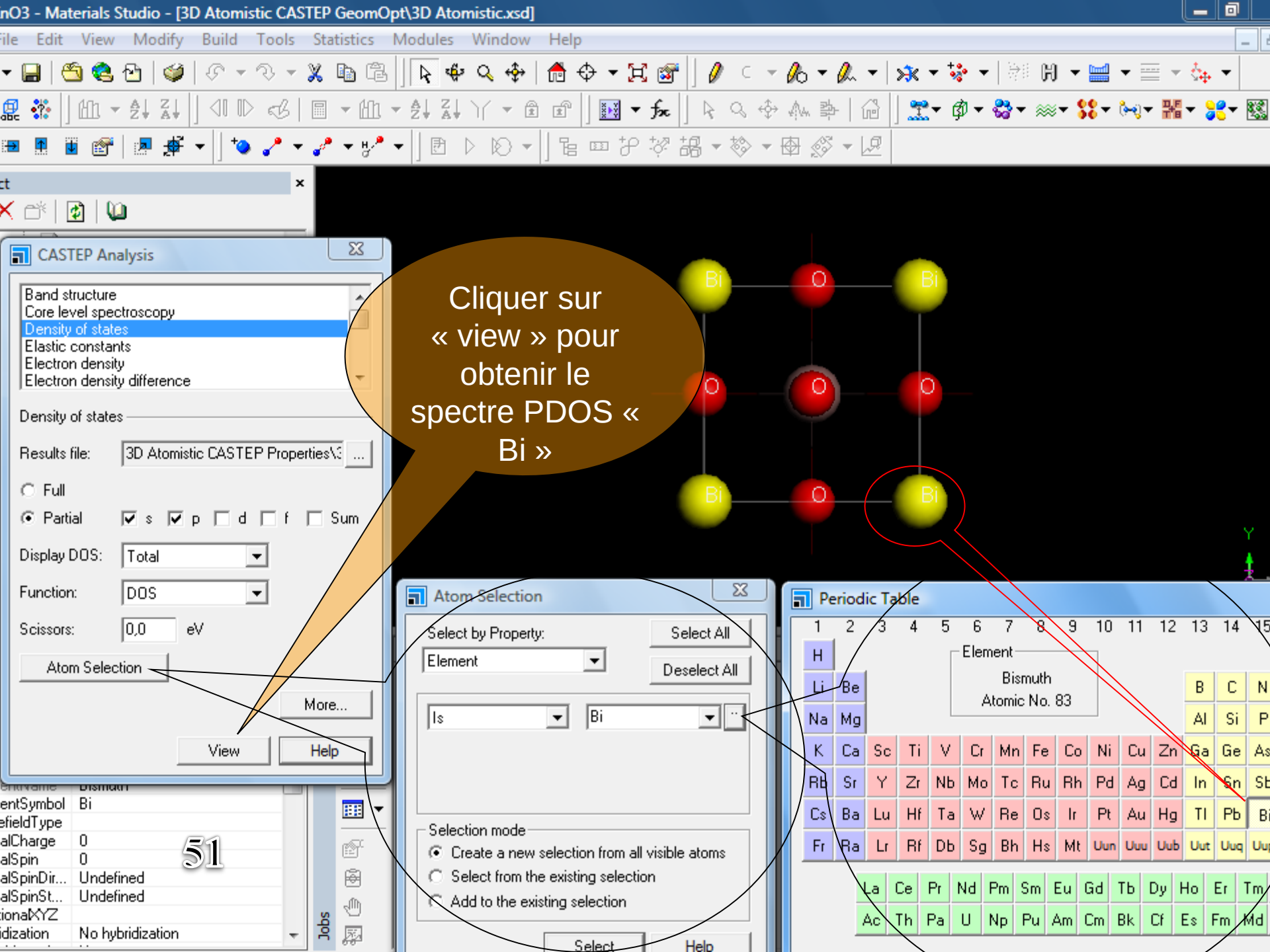


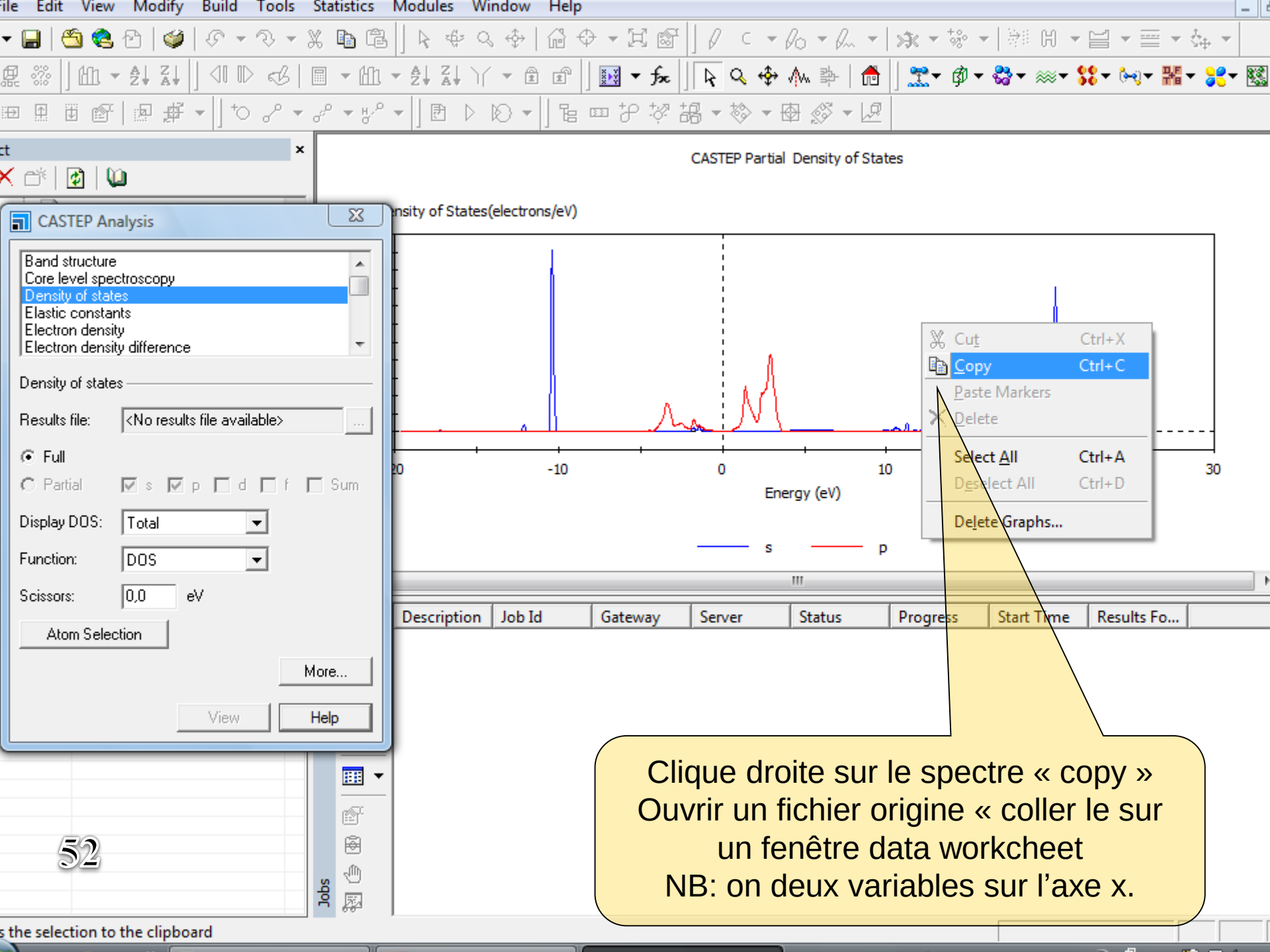
Clique droite sur le spectre « copy »
Ouvrir un fichier origine « coller le sur une fenêtre data worksheet



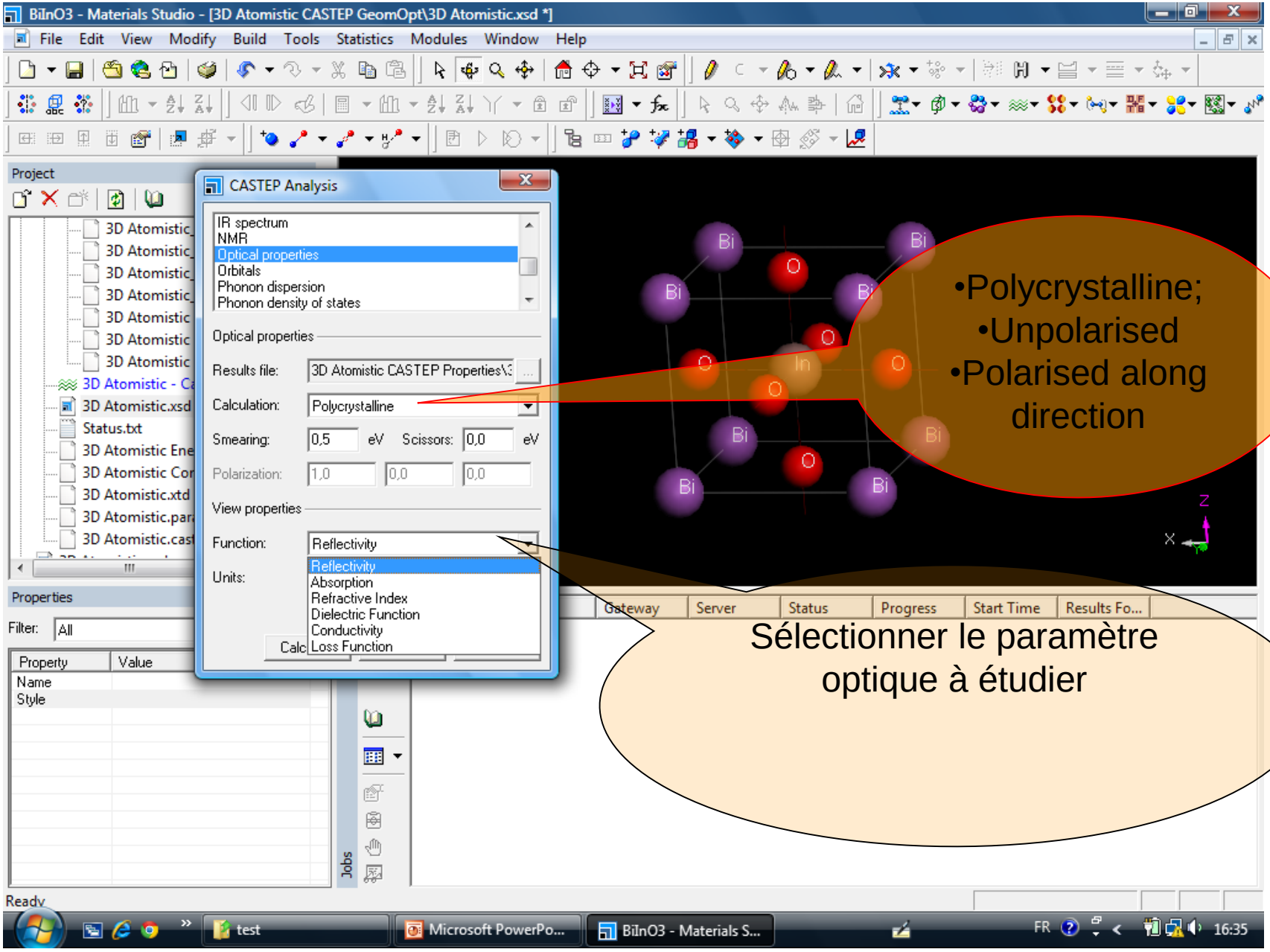
Cliquer sur « view » pour visualiser le spectre TDOS

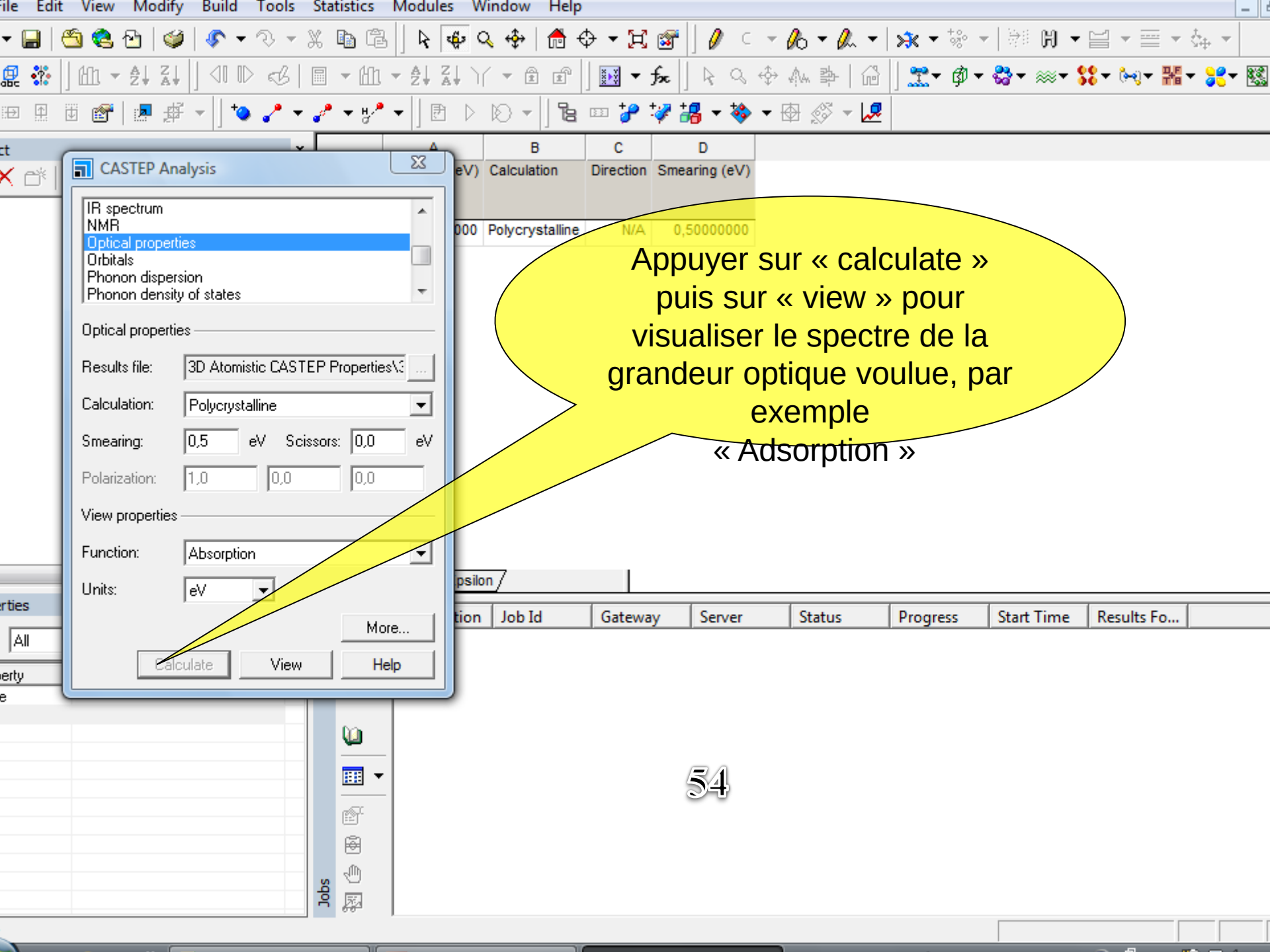

File Edit View Modify Build Tools Statistics Modules Window Help
3D Atomistic - Calculation
Status.txt
3D Atomistic_PopAnl-DensDiff
3D Atomistic_PopAnl-DensDiff
CASTEP Analysis
Band structure
Core level spectroscopy
Density of states
Elastic constants
Electron density
Electron density difference
Density 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
CASTEP Density of States
Density of States(electrons/eV)
40
30
20
10
0
-20
-10
0
10
20
30
Energy (eV)
total
Description
Job Id
Gateway
Server
Status
Progress
Start Time
Results Fo...
Jobs
Clique droite sur le spectre « copy »
Ouvrir un fichier origine « coller le sur un fenêtre data worksheet

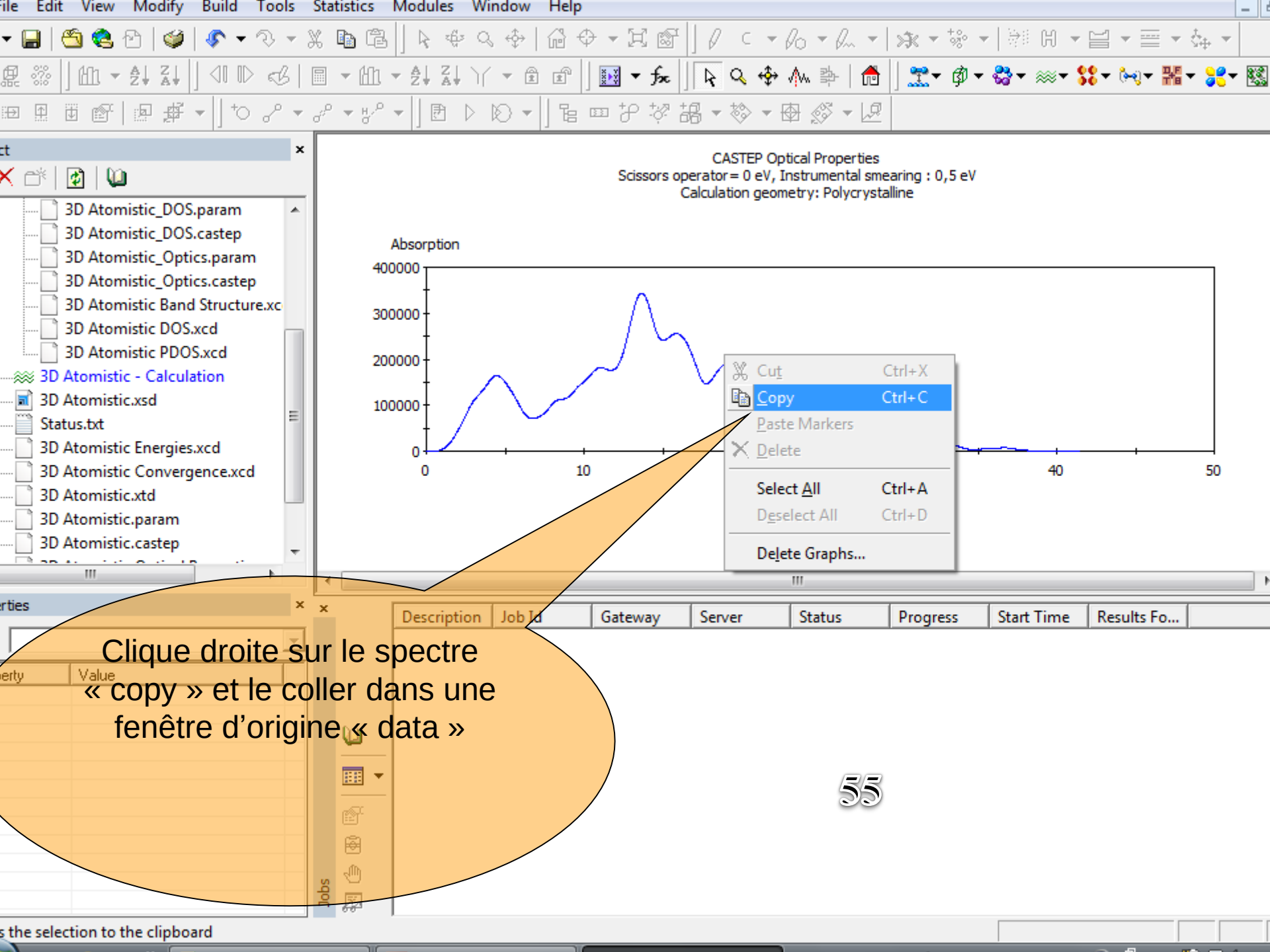

nO3 - Materials Studio - [3D Atomistic CASTEP GeomOpt\3D Atomistic.xsd]
File Edit View Modify Build Tools Statistics Modules Window Help
CASTEP Analysis
Band structure
Core level spectroscopy
Density of states
Elastic constants
Electron density
Electron density difference
Density of states
Results file:
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 »
Bi
O
Atom Selection
Select by Property:
Element
Select All
Deselect All
ls
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
Element
Bismuth
Atomic No. 83
entSymbol Bi
efieldType
alCharge 0
alSpin 0
alSpinDir... Undefined
alSpinSt... Undefined
tionalXYZ
idization No hybridization
51
Jobs


CASTEP Partial Density of States
nsity of States(electrons/eV)
-10
0
10
30
Energy (eV)
s
p
Cut Ctrl+X
Copy Ctrl+C
Paste Markers
Delete
Select All Ctrl+A
Deselect All Ctrl+D
Delete Graphs...
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...
Jobs
s the selection to the clipboard
Clique droite sur le spectre « copy »
Ouvrir un fichier origine « coller le sur
un fenêtre data workcheet
NB: on deux variables sur l'axe x.
52

Analyse des Propriétés optique



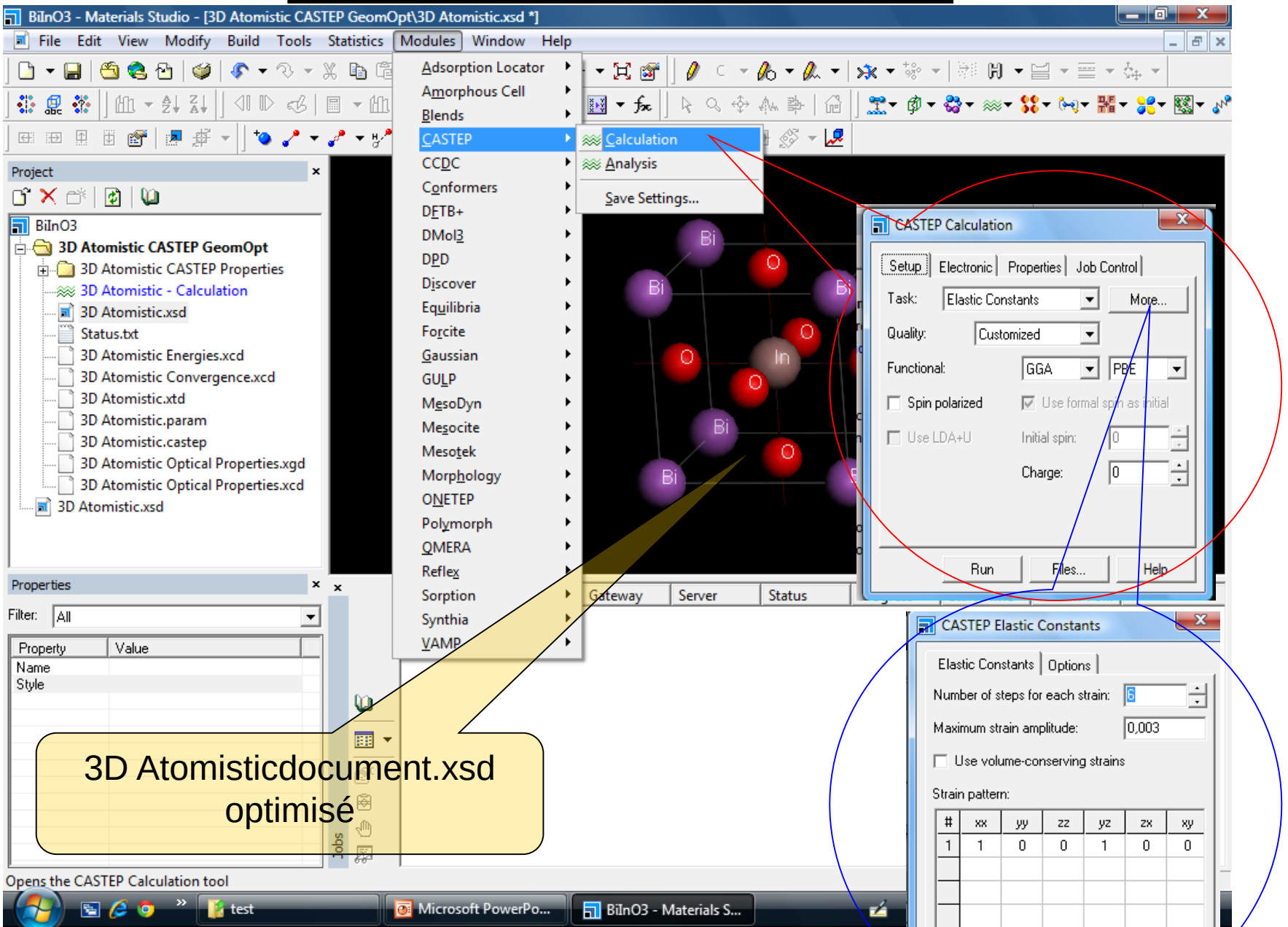

CASTEP Analysis
IR spectrum
NMR
Optical properties
Orbitals
Phonon dispersion
Phonon density of states
Optical properties
Results file:
3D Atomistic CASTEP Properties\3
Calculation:
Polycrystalline
Smearing:
0,5
eV
Scissors:
0,0
eV
Polarization:
1,0
0,0
0,0
View properties
Function:
Absorption
Units:
eV
More...
Calculate
View
Help
B
C
D
Calculation
Direction
Smearing (eV)
Polycrystalline
N/A
0,50000000
Job Id
Gateway
Server
Status
Progress
Start Time
Results Fo...
Jobs
Appuyer sur « calculate »
puis sur « view » pour
visualiser le spectre de la
grandeur optique voulue, par
exemple
« Adsorption »



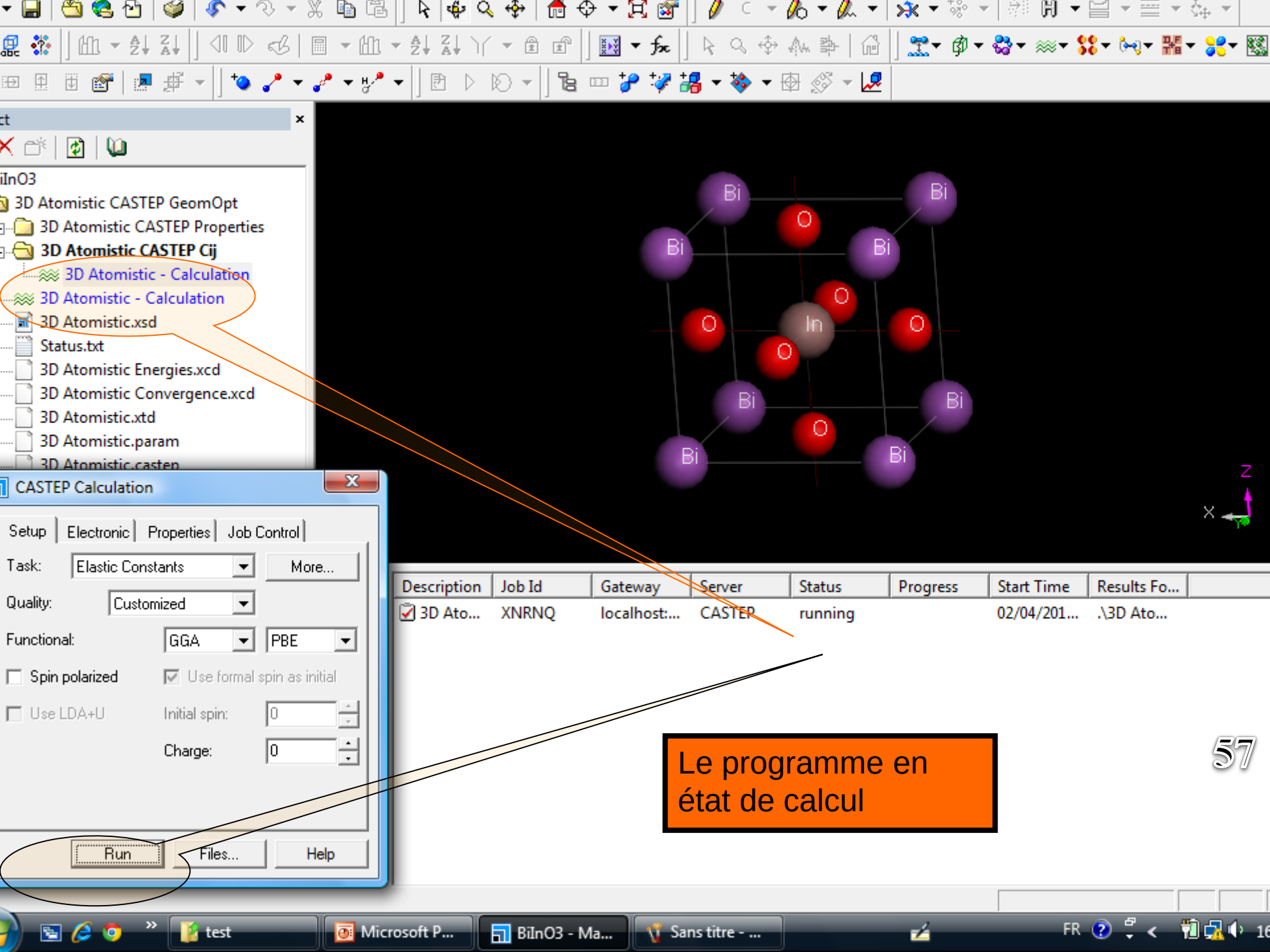
Clique droite sur le spectre « copy » et le coller dans une fenêtre d'origine « data »

Calcul des constants élastiques

« Propriétés élastique »



3D Atomisticdocument.xsd optimisé


iInO3
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
Bi
O
In
CASTEP Calculation
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:
Charge:
Run
Files...
Help
Description
Job Id
Gateway
Server
Status
Progress
Start Time
Results Fo...
3D Ato...
XNRNQ
localhost:...
CASTEP
running
02/04/201...
.\3D Ato...
Le programme en état de calcul
57
test
Microsoft P...
BiInO3 - Ma...
Sans titre - ...
FR

Analyse des constants élastiques