

Material Studio 软件使用简介

Materials Studio 的安装

Materials Studio: Quick Start

Materials Studio 建模

Materials Studio: 计算

Materials Studio: 分析

Material Studio 软件使用简介

2024.04.09

Outline



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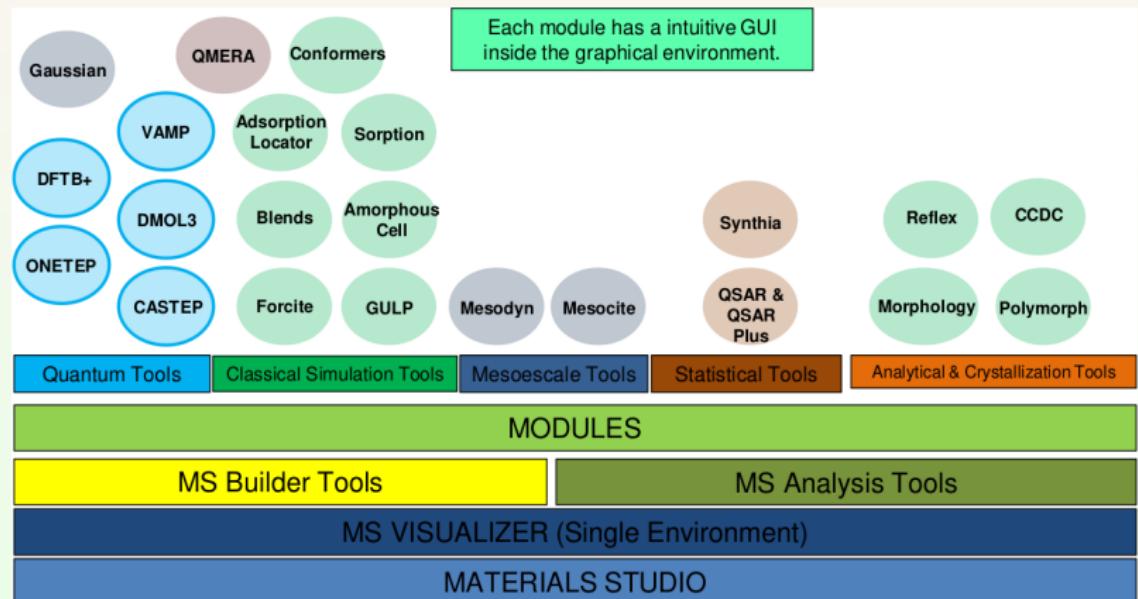


Fig.: The main structure of Materials studio.

MS: Quick Start-01



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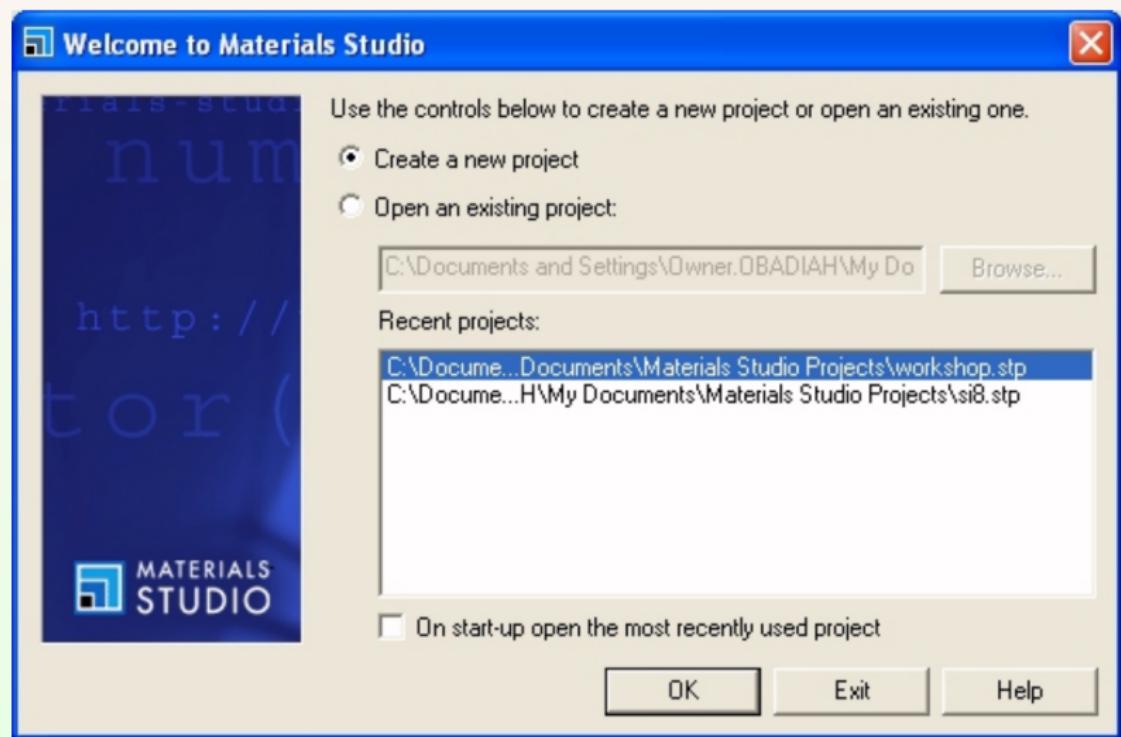


Fig. 1 Quick Start for Materials studio Step 01

MS: Quick Start-02

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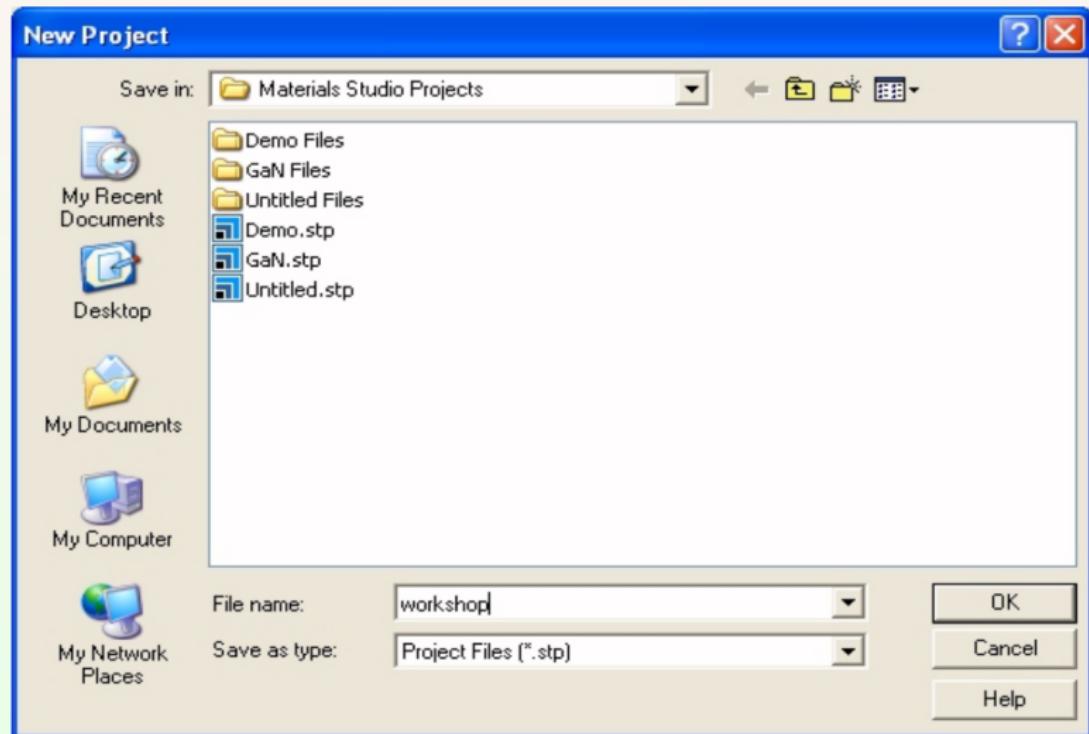


Fig.: Quick Start for Materials studio: Step-02.

MS: Quick Start-03

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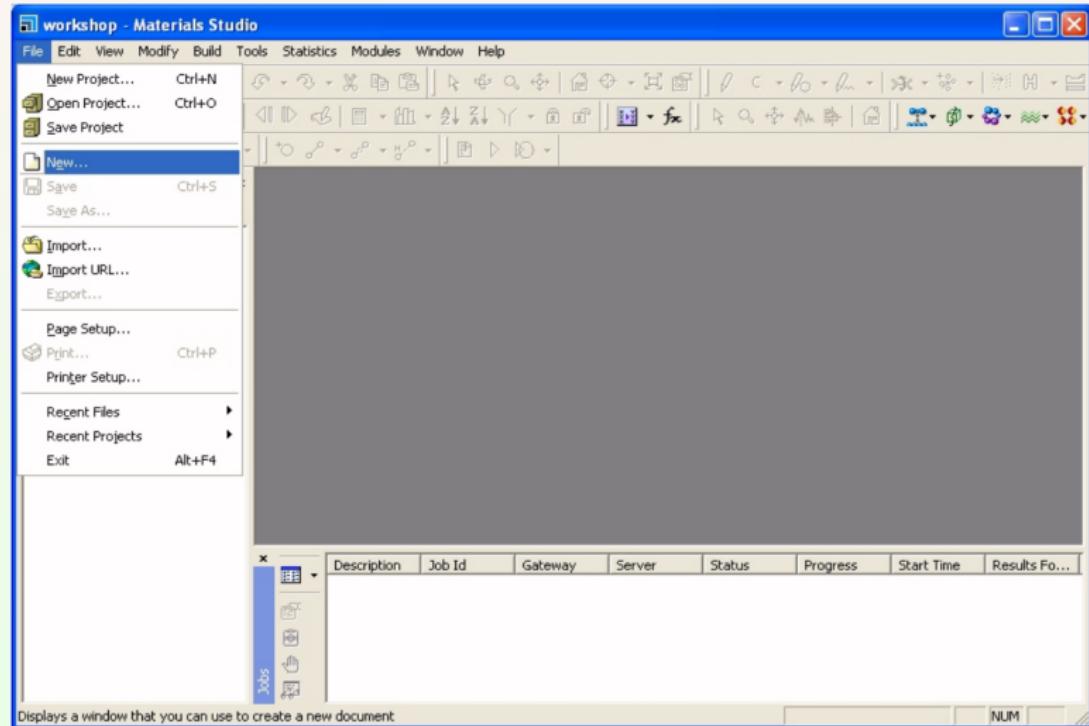


Fig.: Quick Start for Materials studio: Step-03. 

MS: Quick Start-Modelling-01

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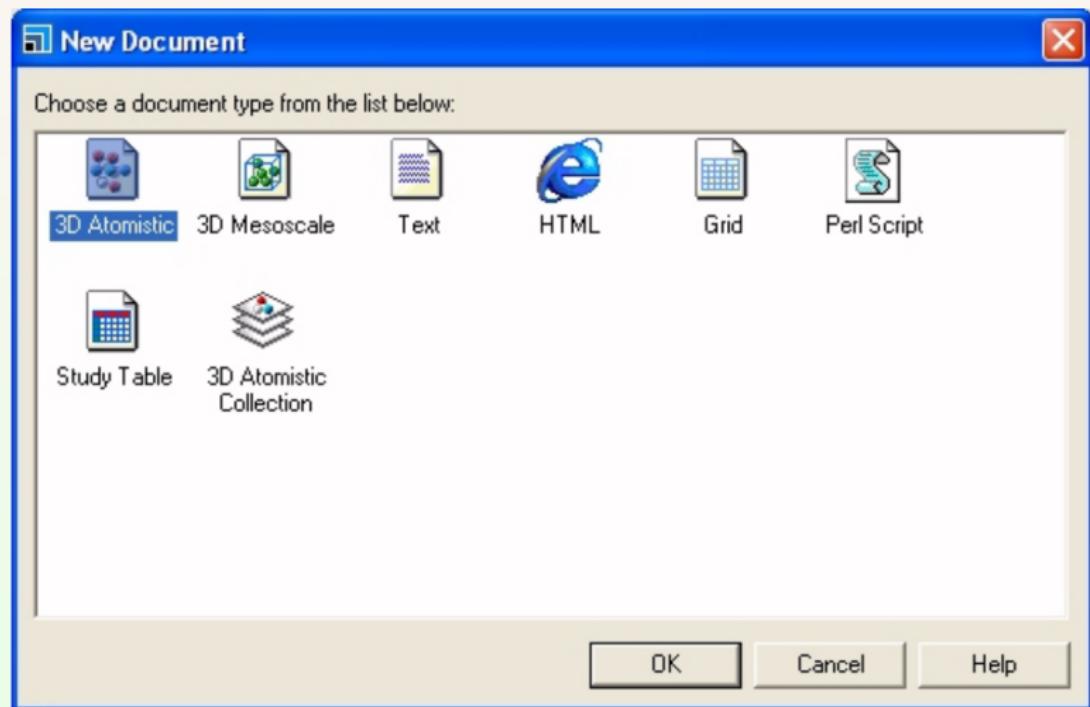


Fig.: Quick Start for Materials studio: Modelling-01.

MS: Quick Start-Modelling-02

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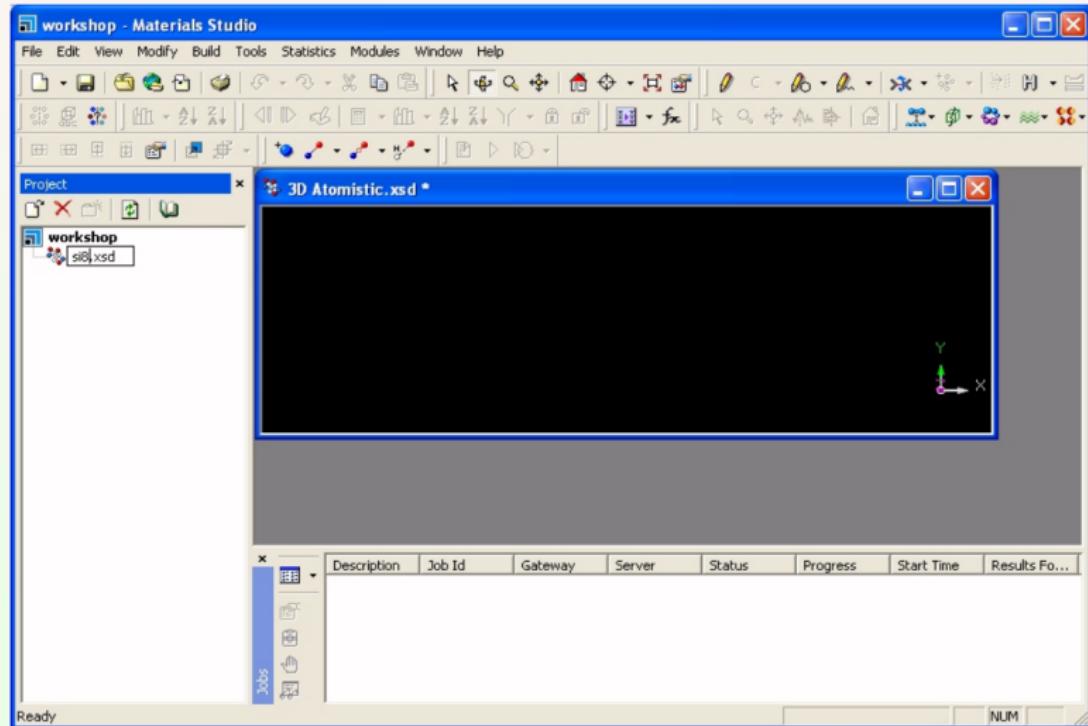


Fig.: Quick Start for Materials studio: Modelling-02.

MS: Modelling Crystal-01

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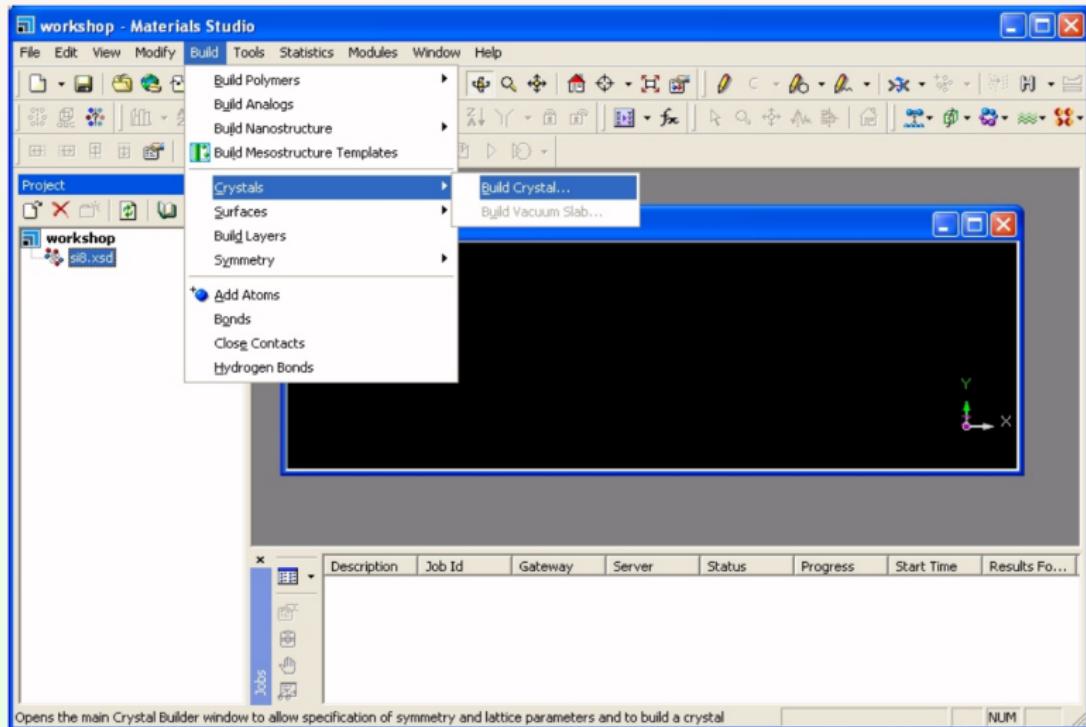


Fig.: Modelling crystal by Materials studio.

MS: Modelling Crystal-02



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The screenshot shows the 'Build Crystal' dialog box with the following details:

- Space Group:** fd3m
- Option:** Origin-1
- Space group information:**

Name	P1
IT Number	1
Option	Origin-1
Long Name	P1
Schoenflies Name	C1-1
Crystal System	Triclinic
Crystal Class	1
Primitive-Centered	(0,0,0)
# of Operators	1
- Operators:** A table showing the operator 1 with components x, y, and z.
- Buttons:** Build, Apply, Cancel, Help, Details...

Fig.: Modelling crystal by Materials studio: Parameters.

MS: Modelling Crystal-03

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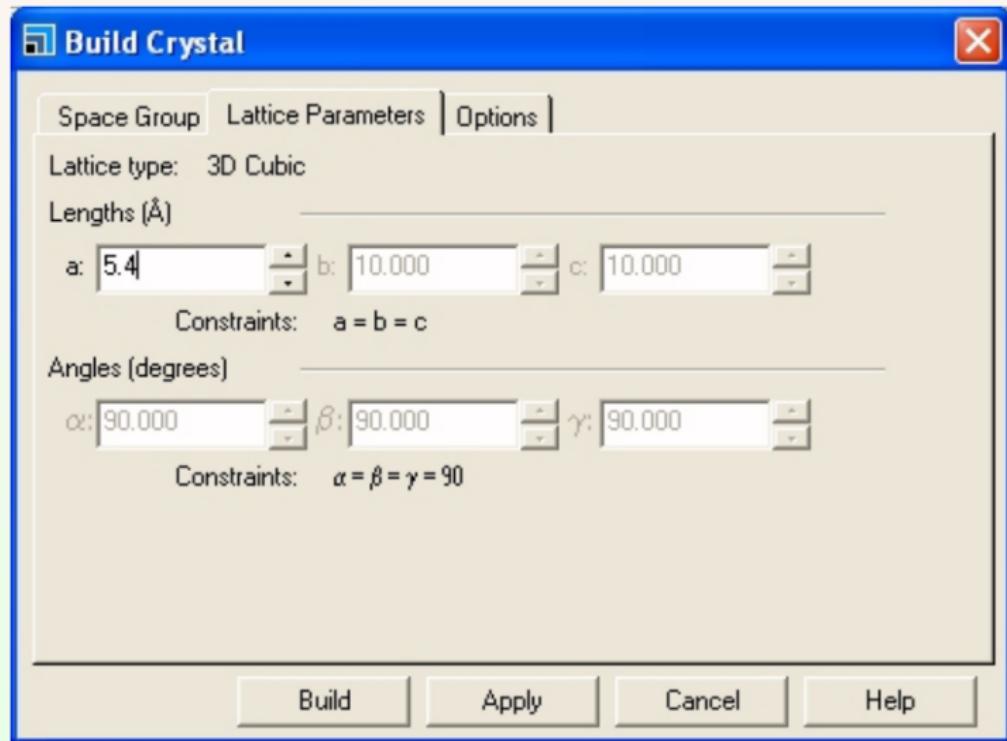


Fig.: Modelling crystal by Materials studio: Lattice parameters.

MS: Modelling Crystal-04

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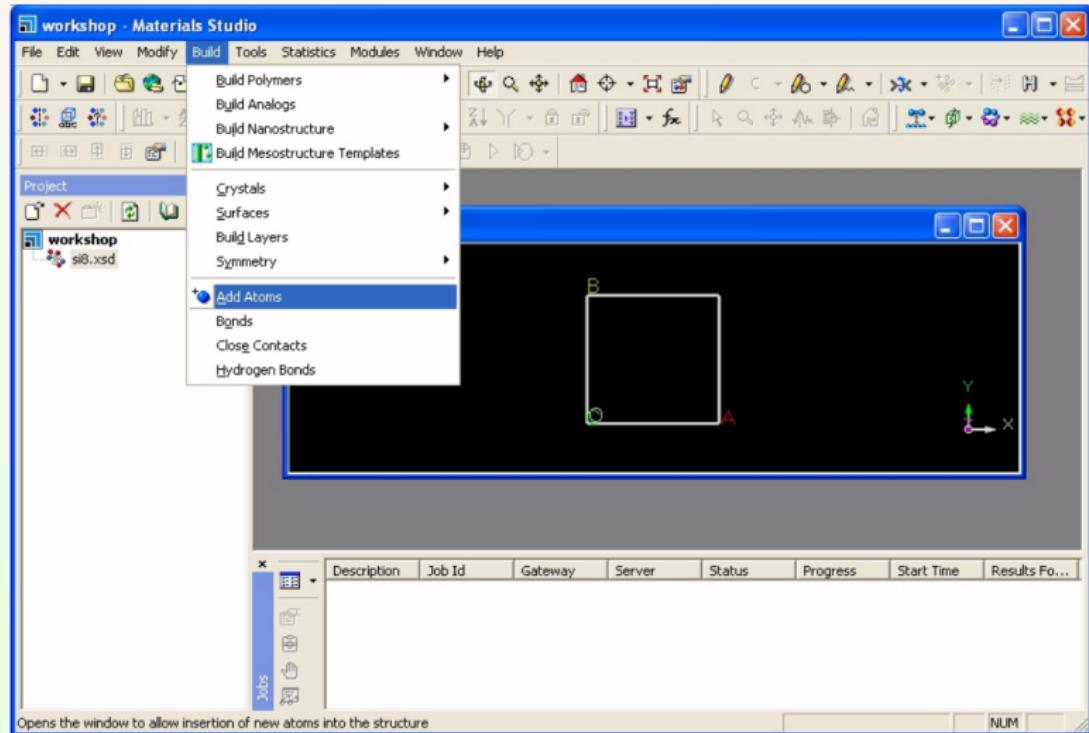


Fig.: Modelling crystal by Materials studio: Elements.

MS: Modelling Crystal example: Si

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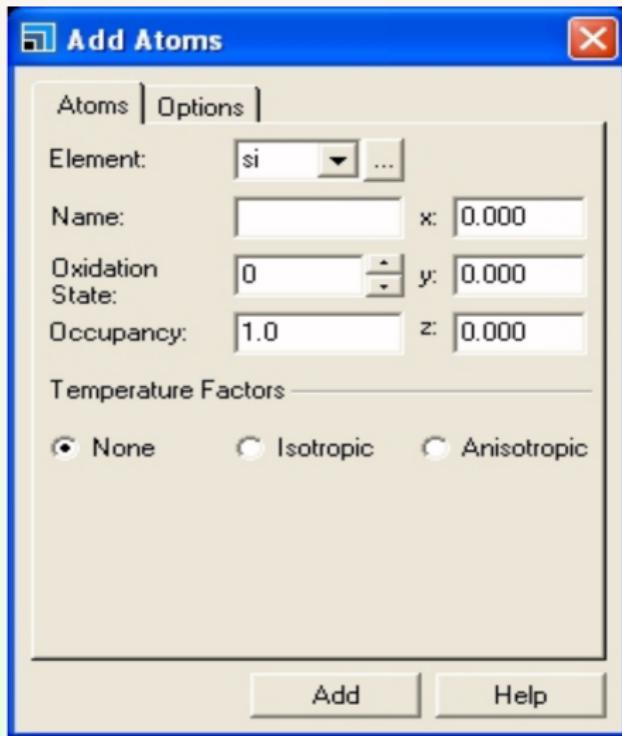


Fig.: Modelling crystal by Materials studio: Si.

MS: Modelling Crystal example: Si



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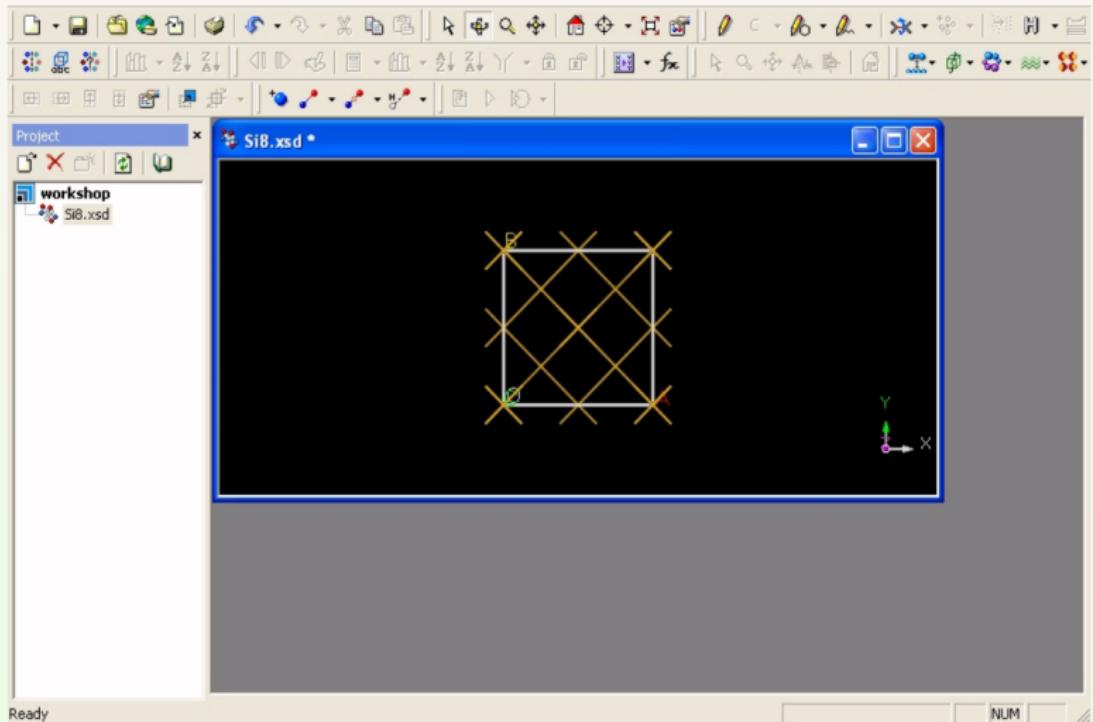


Fig.: Modelling crystal by Materials studio: Si.

MS: CASTEP Calculation example: Si

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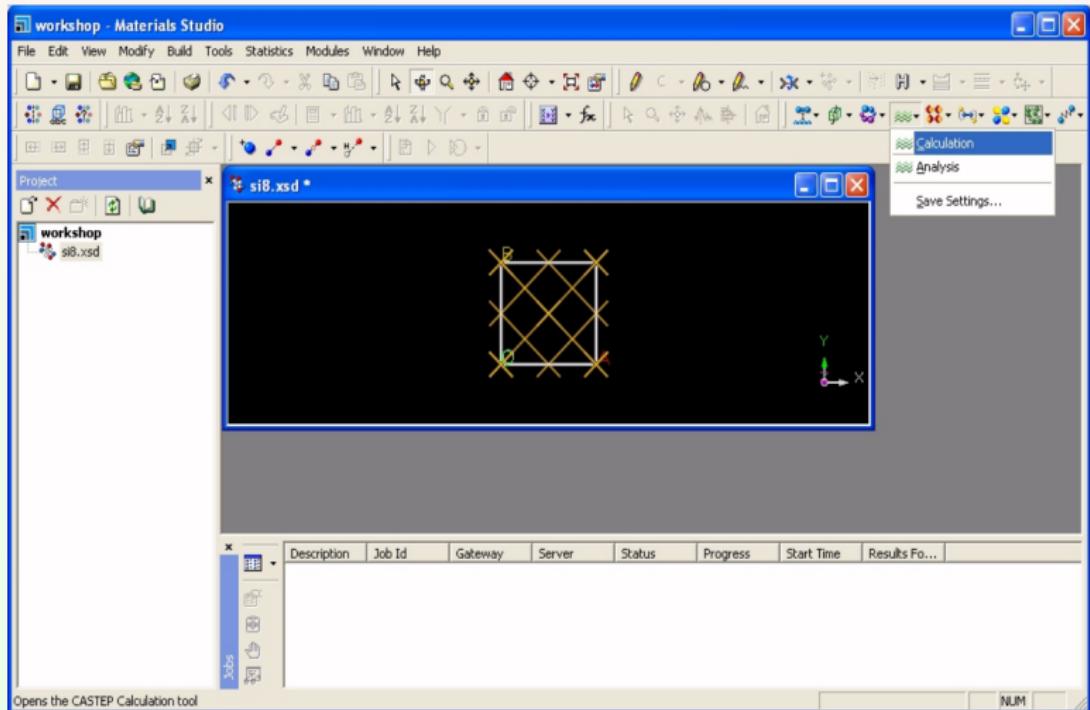


Fig.: CASTEP Calculation by Materials studio: Si.

MS: CASTEP Calculation example: Si

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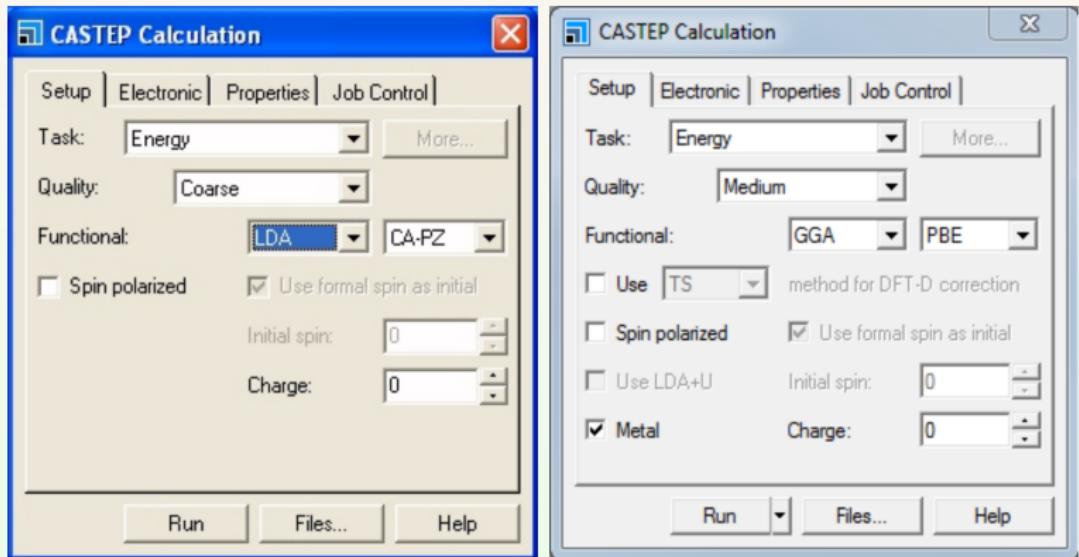


Fig.: CASTEP Calculation by Materials studio: Parameter.

MS: CASTEP Calculation example: Si

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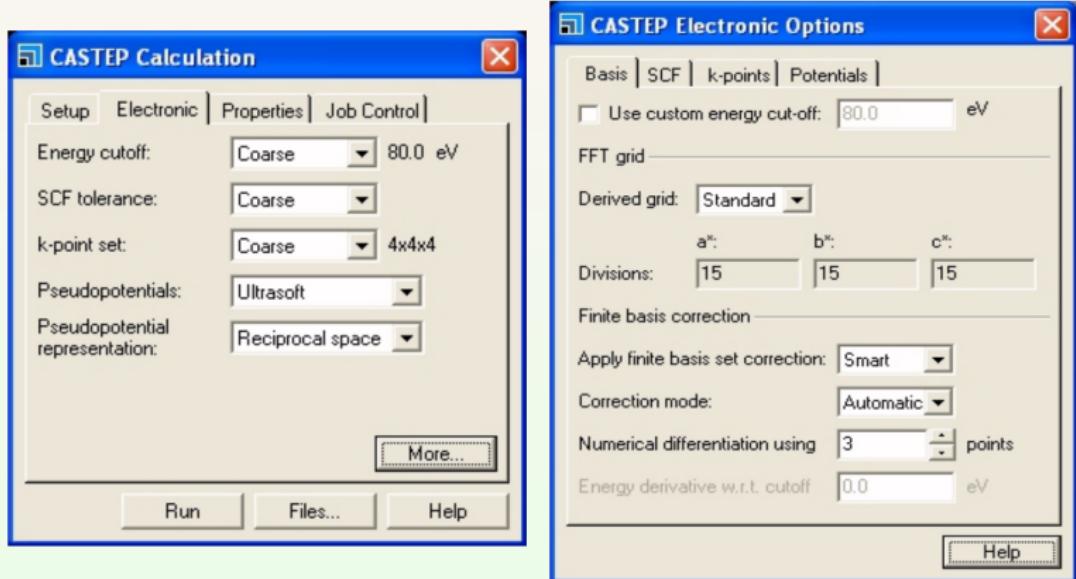


Fig.: CASTEP Calculation by Materials studio: Electron-step.

MS: CASTEP Calculation example: Si



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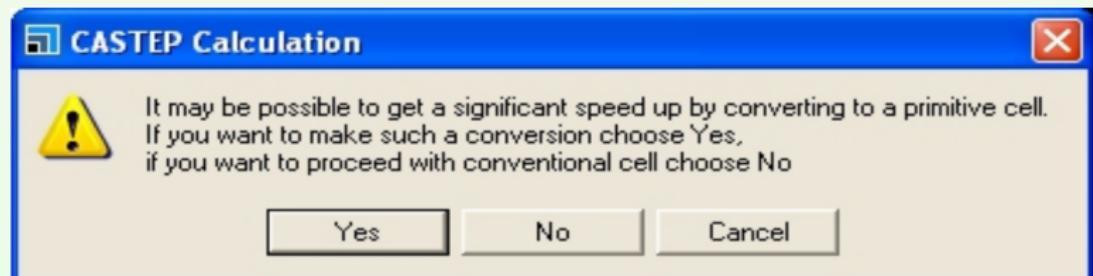
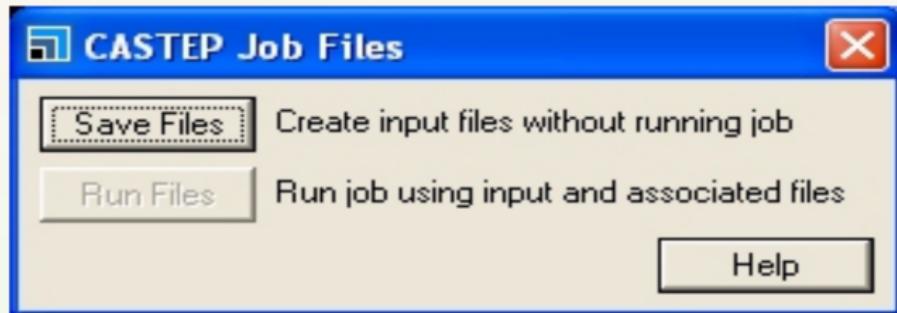


Fig.: CASTEP Calculation.

MS: CASTEP Calculation example: Si

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Fig.: CASTEP Calculation by Materials studio: Connect to localhost,

MS: CASTEP Calculation example: Si

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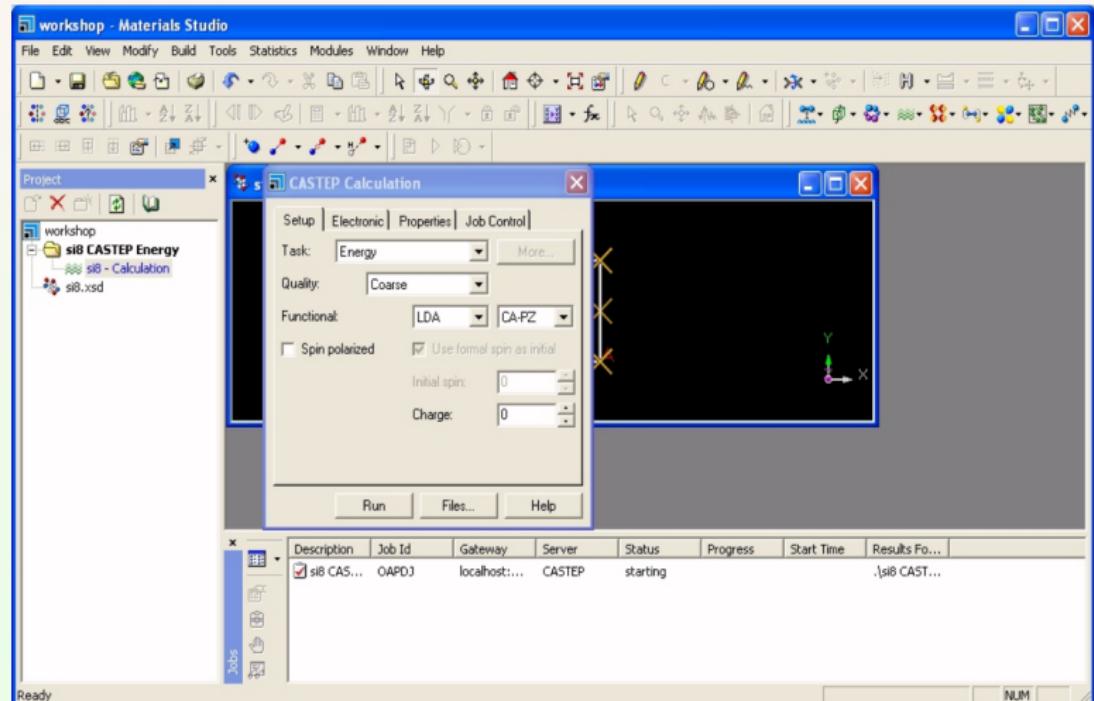


Fig.: CASTEP Calculation by Materials studio: Run.

MS: CASTEP Calculation example: Si



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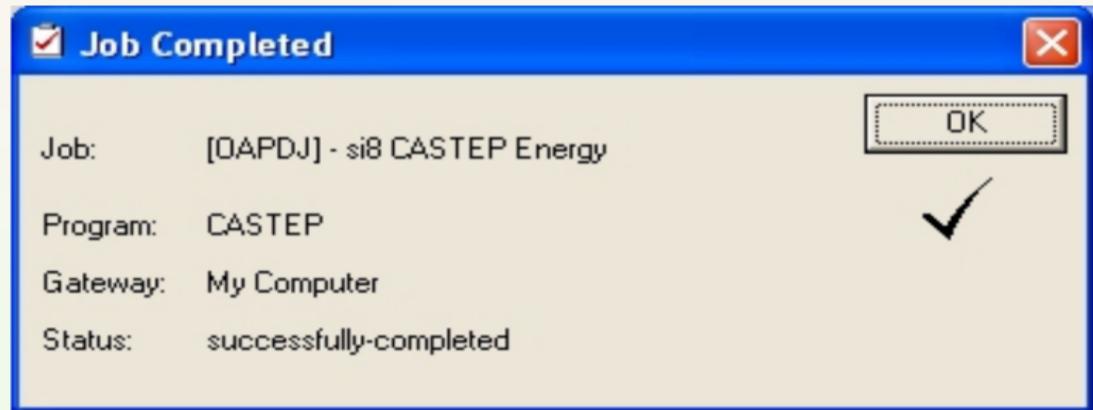


Fig.: CASTEP Calculation by Materials studio: Complete.

MS: CASTEP Calculation example: Si

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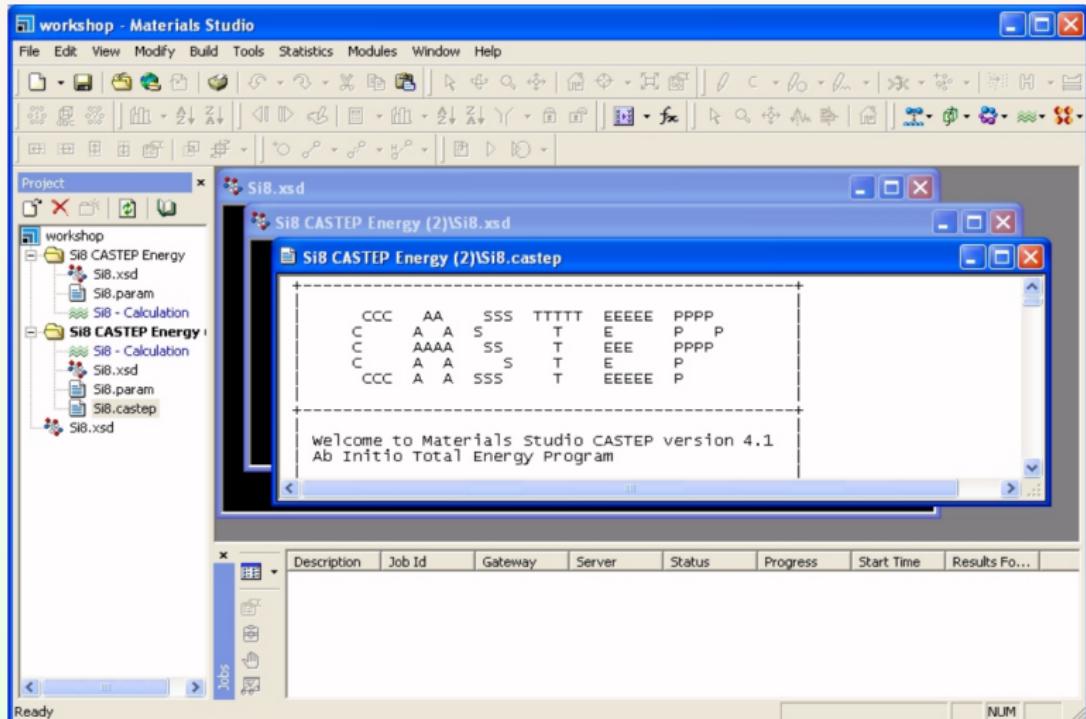


Fig.: CASTEP Calculation by Materials studio; Finish.

MS: CASTEP Calculation example: Si

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```

----- <-- SCF
SCF loop      Energy          Fermi          Energy gain      Timer   <-- SCF
                           energy          per atom      (sec)    <-- SCF
----- <-- SCF
Initial     2.11973065E+002  4.85767974E+001           0.61  <-- SCF
Warning: There are no empty bands for at least one kpoint and spin; this may
         slow the convergence and/or lead to an inaccurate groundstate.
         If this warning persists, you should consider increasing nextra_bands
         and/or reducing smearing_width in the param file.
         Recommend using nextra_bands of 7 to 15.

          1 -7.22277610E+002  1.02240172E+001  1.16781334E+002  0.88  <-- SCF
          2 -8.53739673E+002  6.90687627E+000  1.64327579E+001  1.12  <-- SCF
          3 -8.62681938E+002  6.65069587E+000  1.11778315E+000  1.39  <-- SCF
          4 -8.62169156E+002  6.69758744E+000  -6.40977798E-002  1.72  <-- SCF
          5 -8.61880601E+002  6.78641872E+000  -3.60693332E-002  2.06  <-- SCF
          6 -8.61884687E+002  6.79549194E+000  5.10791707E-004  2.44  <-- SCF
          7 -8.61884645E+002  6.79874201E+000  -5.25062118E-006  2.75  <-- SCF
          8 -8.61884639E+002  6.79822409E+000  -8.40318139E-007  2.98  <-- SCF
----- <-- SCF

Final energy, E      = -861.8846385210      eV
Final free energy (E-TS) = -861.8846385210      eV
(energies not corrected for finite basis set)

NB est. OK energy (E-0.5TS)      = -861.8846385210      eV

```

Fig.: CASTEP Calculation by Materials studio: SCF.

MS: CASTEP Analysis example: Si

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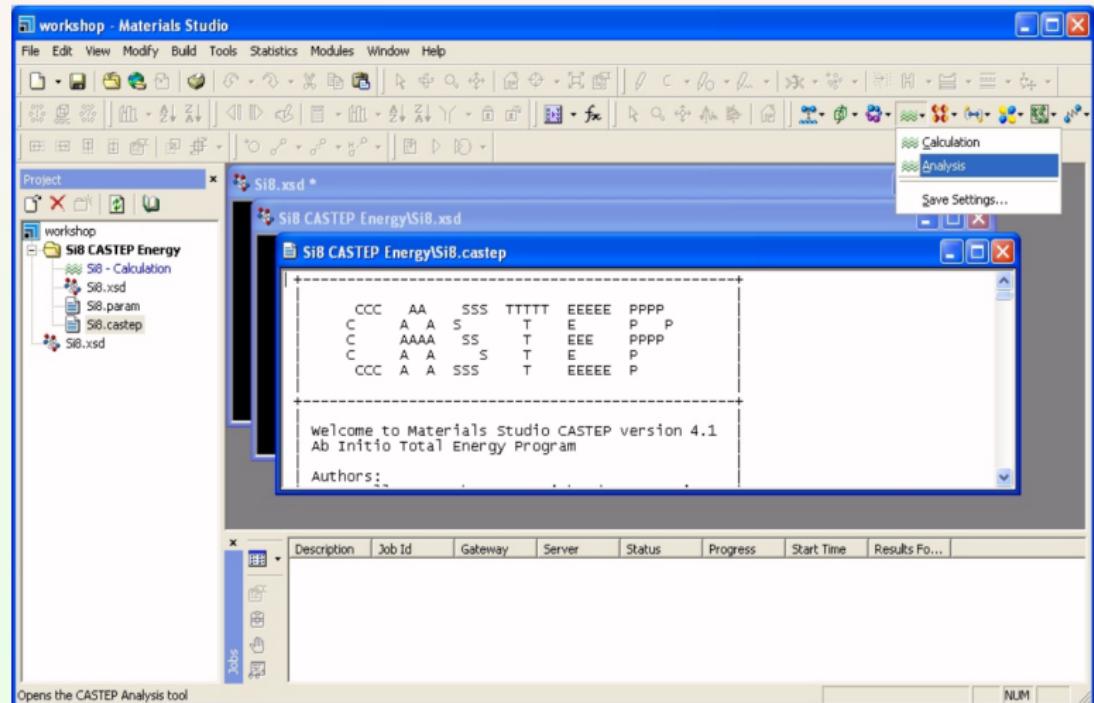


Fig.: CASTEP Analysis by Materials studio.

MS: CASTEP Analysis example: Si

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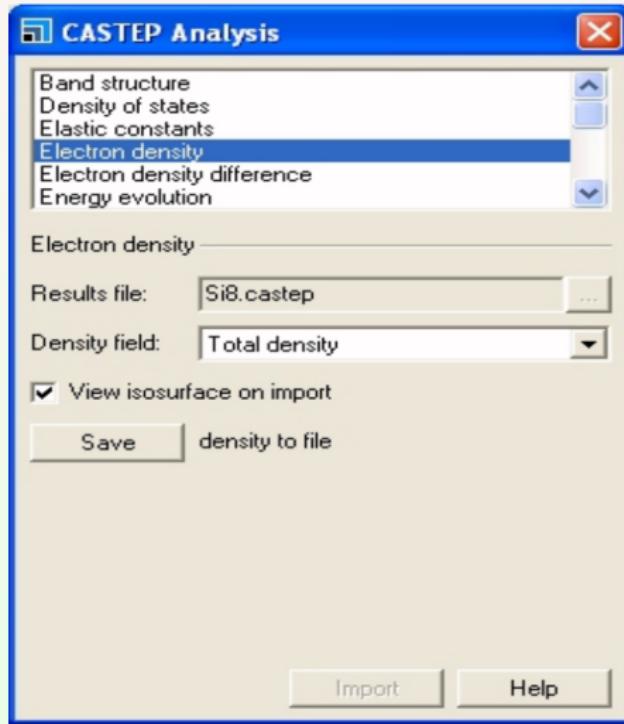


Fig.: CASTEP Analysis by Materials studio: Parameter,

MS: CASTEP Analysis example: Si

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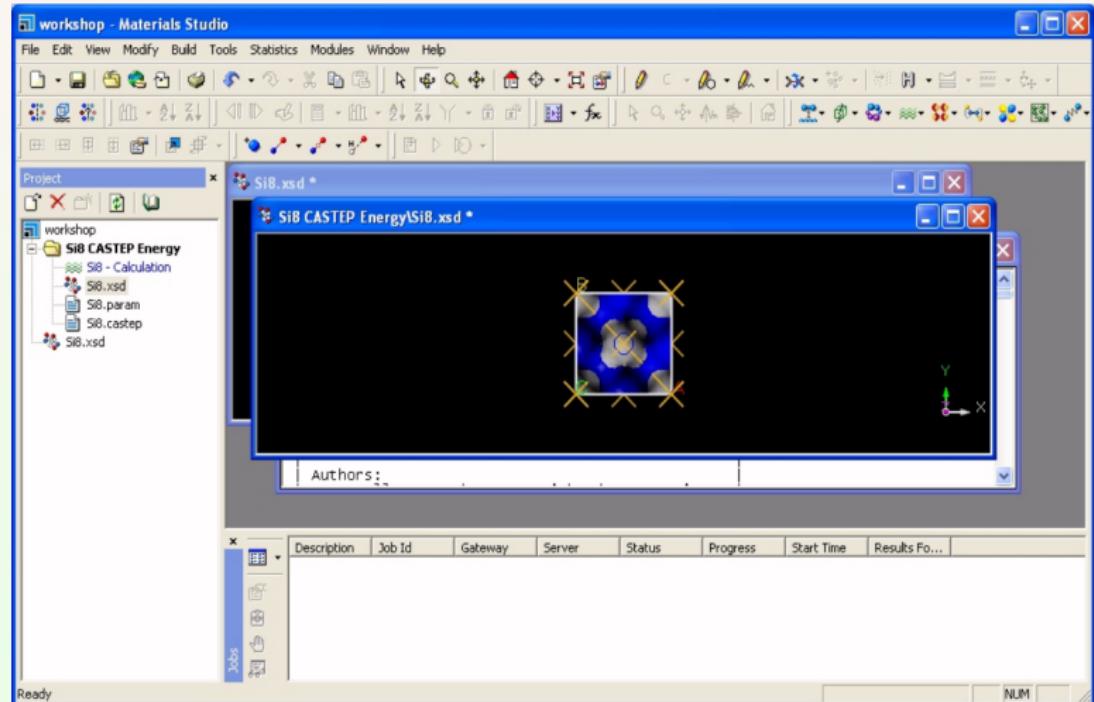


Fig.: CASTEP Analysis by Materials studio: Charge.

MS: CASTEP Analysis example: Si

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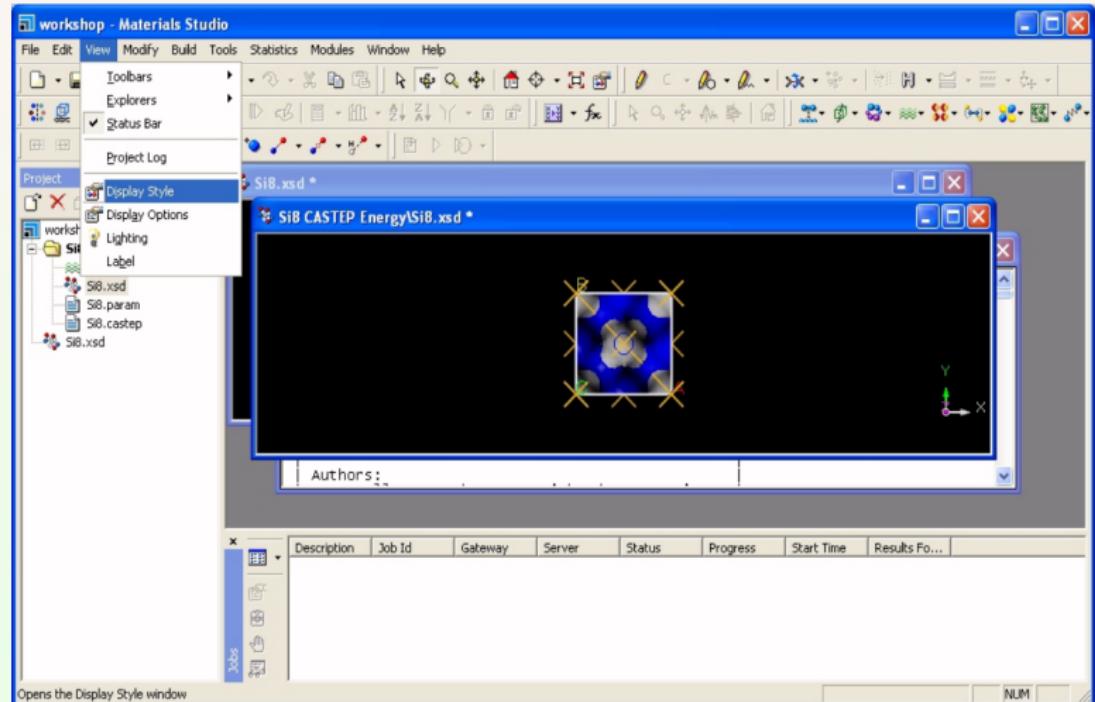


Fig.: CASTEP Analysis by Materials studio: Display-style.

MS: CASTEP Analysis example: Si

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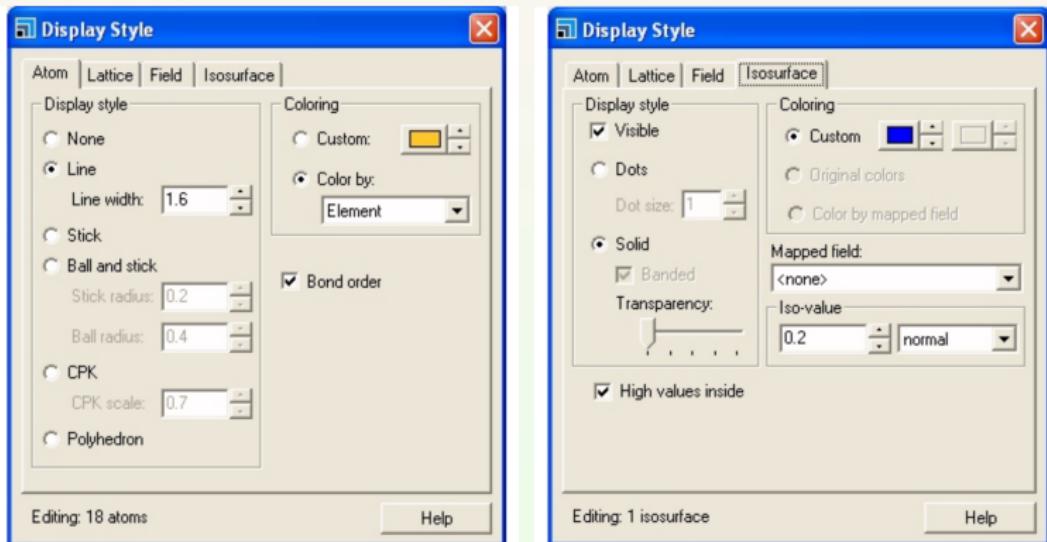


Fig.: CASTEP Analysis by Materials studio: Display-parameter.

MS Modelling: Polymers

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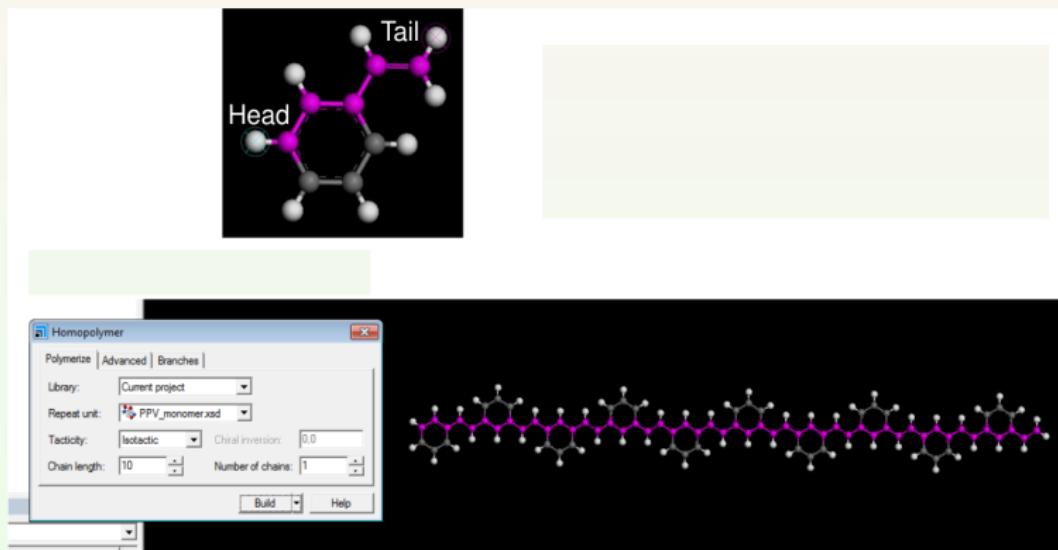


Fig.: Building homopolymer for Materials studio.

MS Modelling: Polymers

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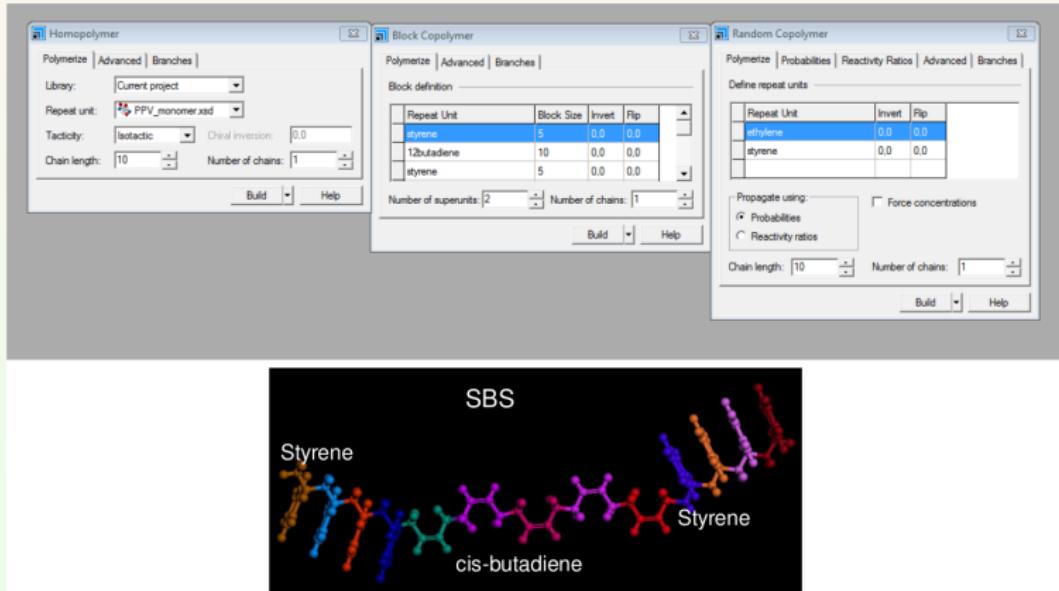


Fig.: Building multi-polymer for Materials studio.

MS Modelling: amidoamine

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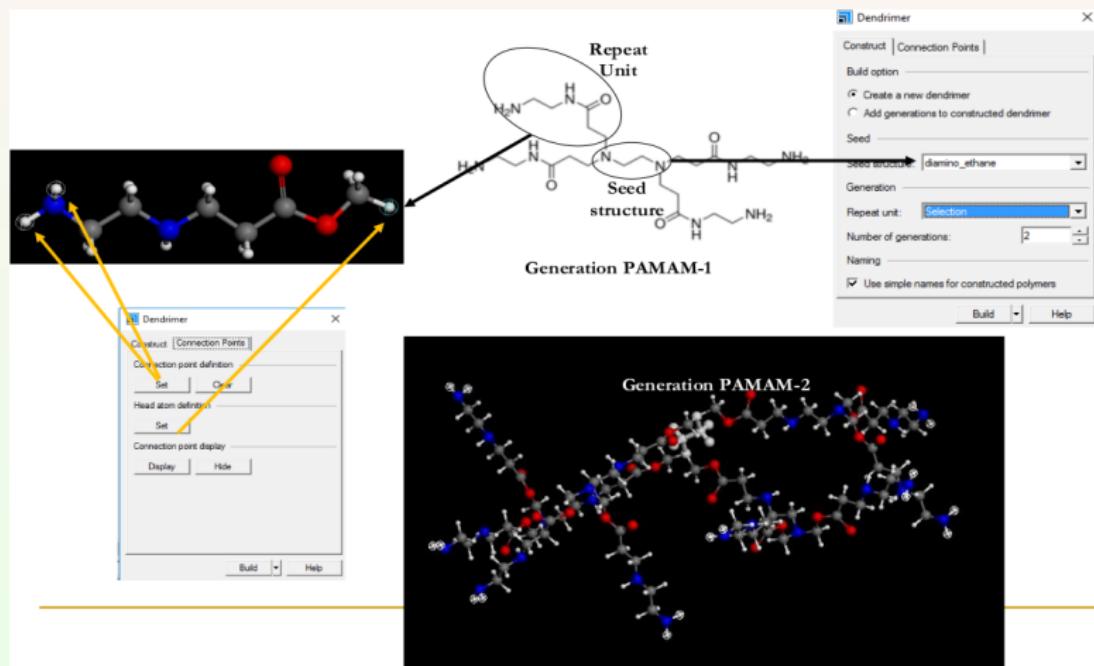


Fig.: Building Poly-amidoamine (PAMAM) for Materials studio.

MS Modelling: from similar



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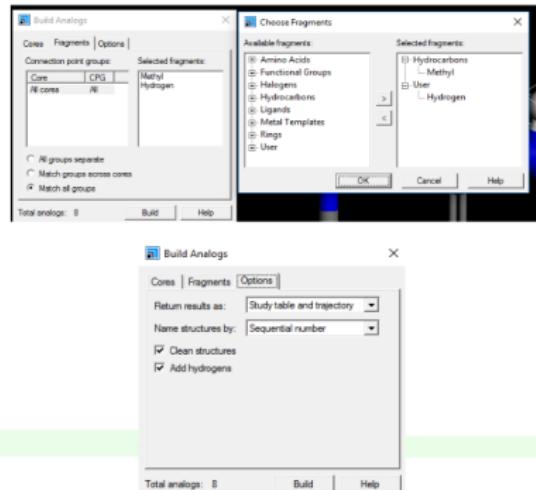
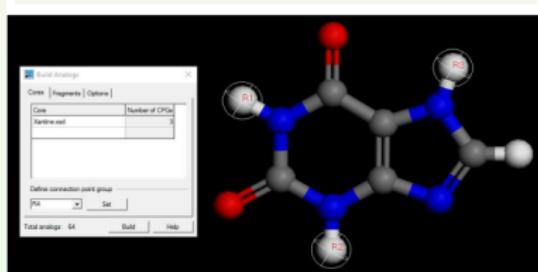
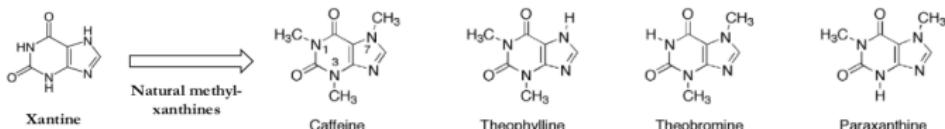


Fig.: Building from similar structure for Materials studio.

MS Modelling: from similar

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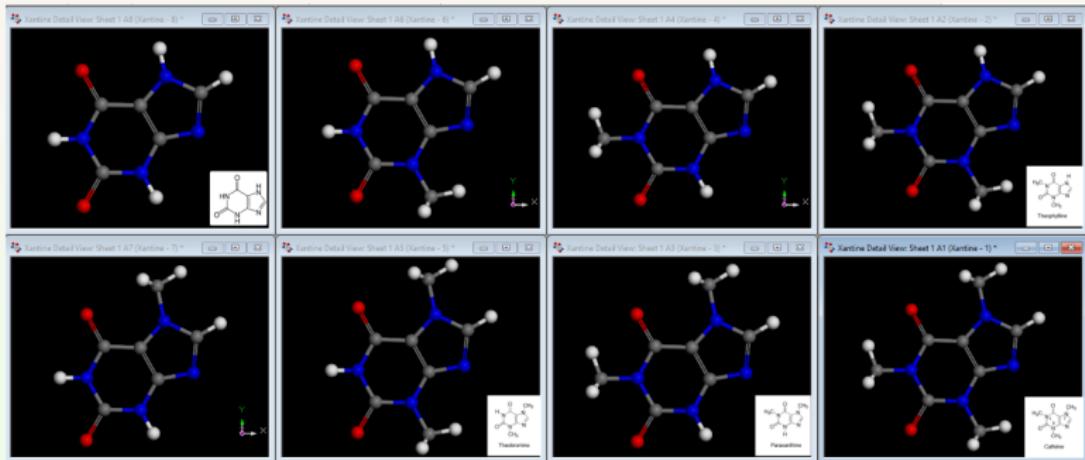


Fig.: The similar structures in Materials studio.

MS Modelling: Single-wall Nanotubes

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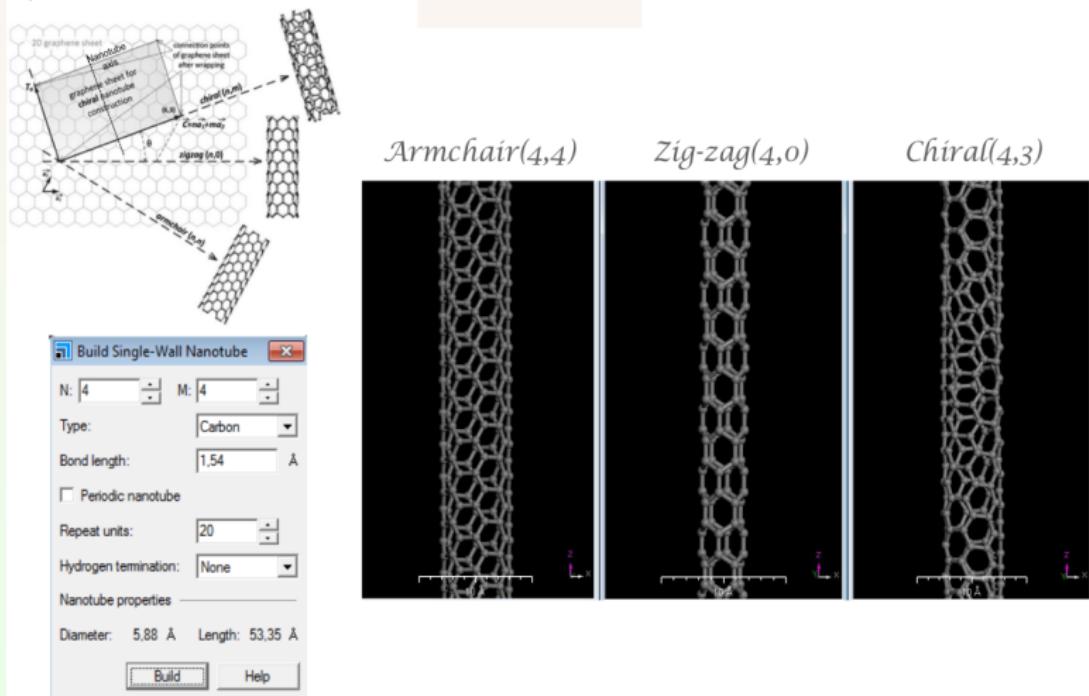


Fig.: Building Single-wall Nanotubes for Materials studio.

MS Modelling: Single-wall Nanotubes

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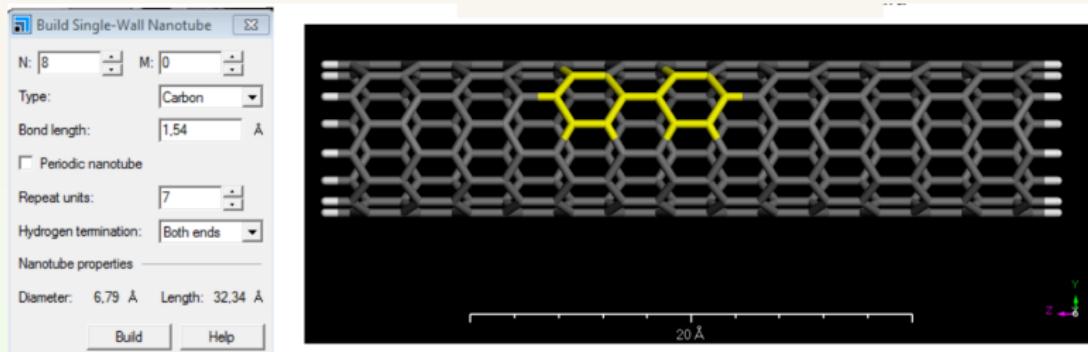


Fig.: Building Single-wall Nanobubes: Select atoms for Materials studio.

MS Modelling: Multi-wall Nanotubes



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The nanotubes will be rotated relative to one another in order to minimize the strain energy

$$E_{strain} = -\frac{A}{r^6} + \frac{B}{r^{12}}$$
$$A = 77.15 eV\text{\AA}^6, B = 1.14548 \times 10^5 eV\text{\AA}^{12}$$

Zhang, et al. . Phys. Rev. B, 70, 035403 (2004).

Fig.: Building Multi-wall Nanotubes for Materials studio.

MS Modelling: Single-wall Nanotubes bundle

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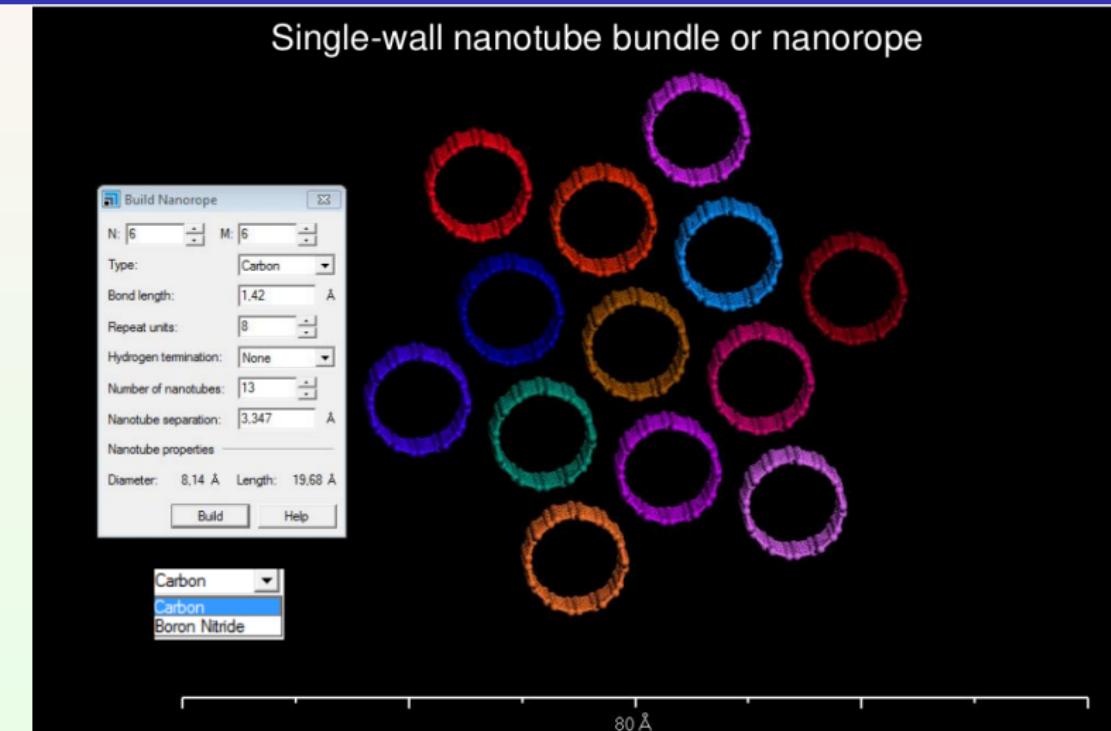


Fig.: Building Single-wall Nanotube bundle or nanorope for Materials studio.

MS Modelling: Construction of Nanocluster



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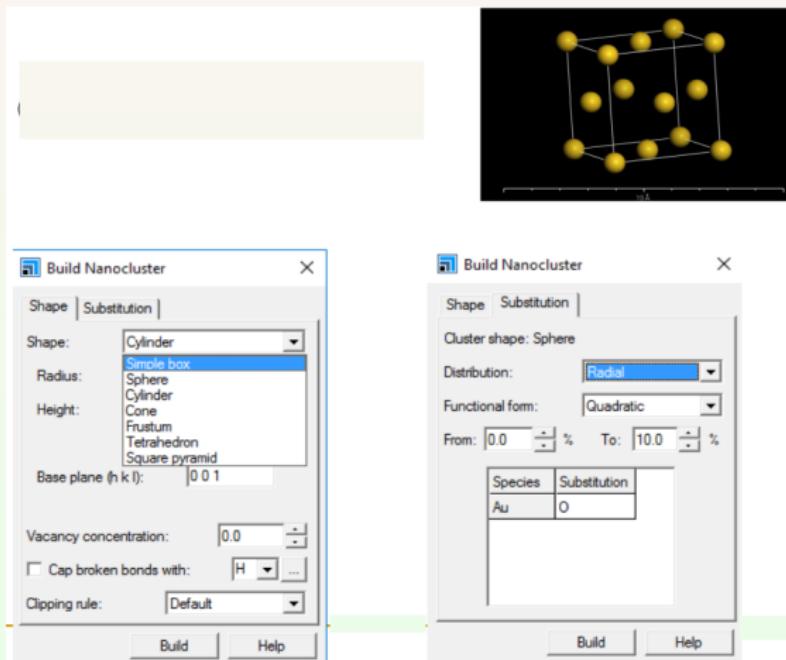


Fig.: Building of Nanocluster for Materials studio.

MS Modelling: Construction of Nanocluster

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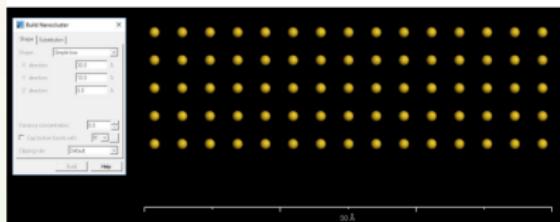
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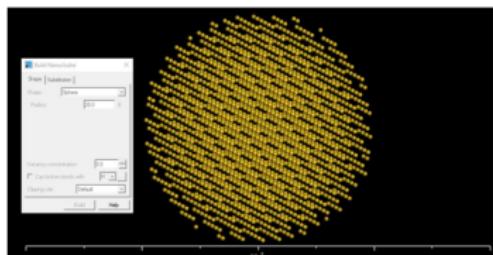
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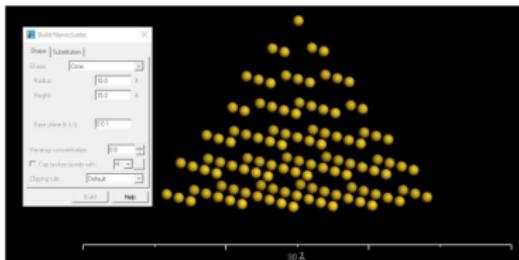
Au Nanocluster. Single Box



Au Nanocluster. Sphere



Au Nanocluster. Cone



Au Nanocluster. Sphere. Ag substitution

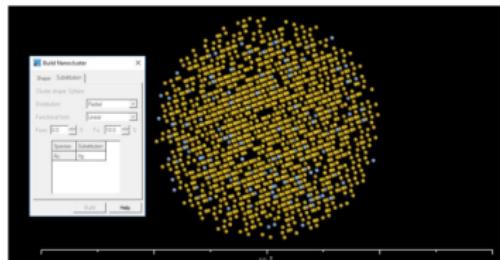


Fig.: The Nanocluster structures in Materials studio.

MS Modelling: Meso-molecules

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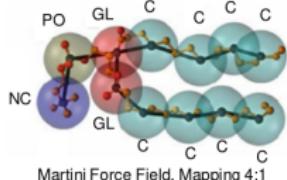
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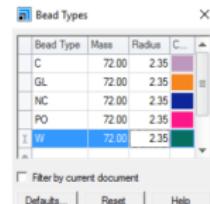
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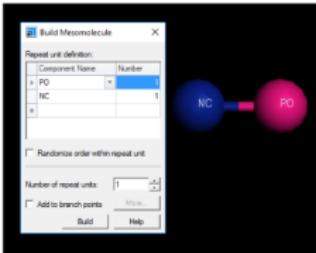
Dipalmitoylphosphatidylcholine (DPPC)



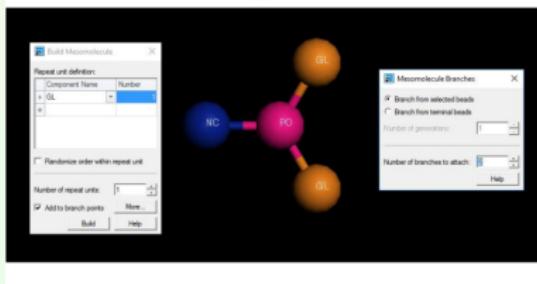
Defining the CG beads



Building the head



Positioning the GL beads



Building the tails

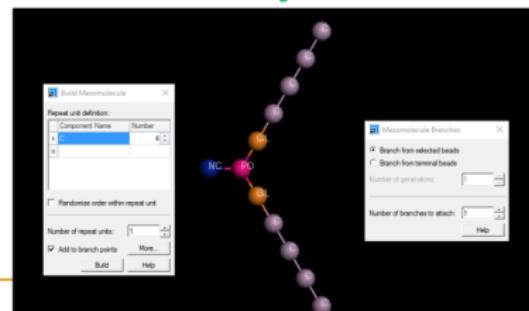


Fig.: Building Meso-molecule structure for Materials studio.

MS Modelling: Meso-molecules by template



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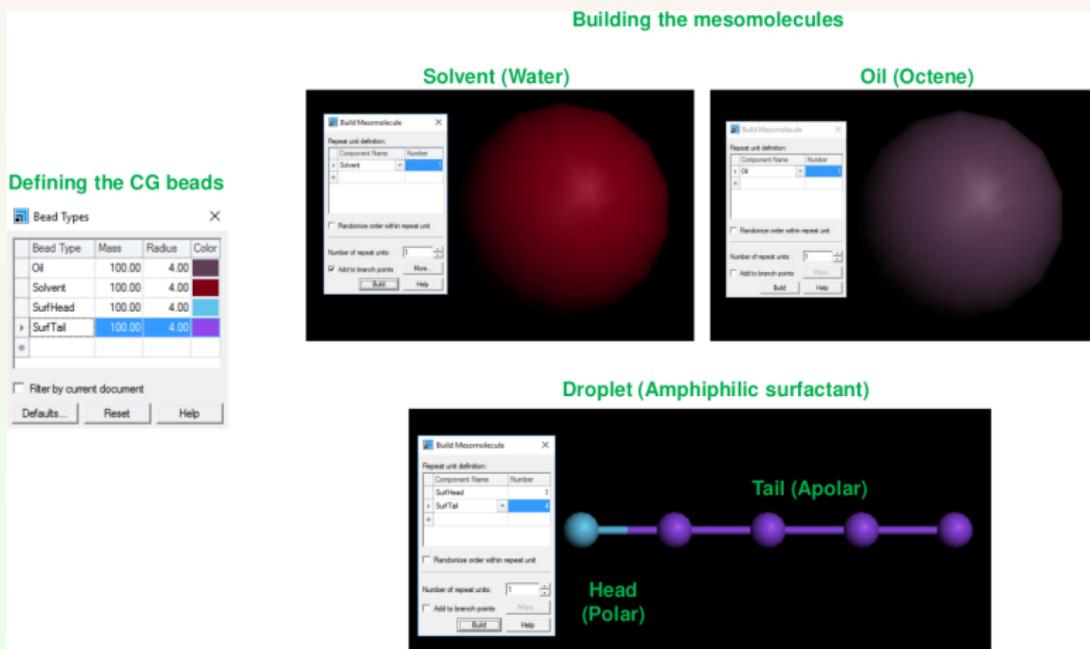


Fig.: Building Meso-molecule by template for Materials studio.

MS Modelling: Meso-molecules by template

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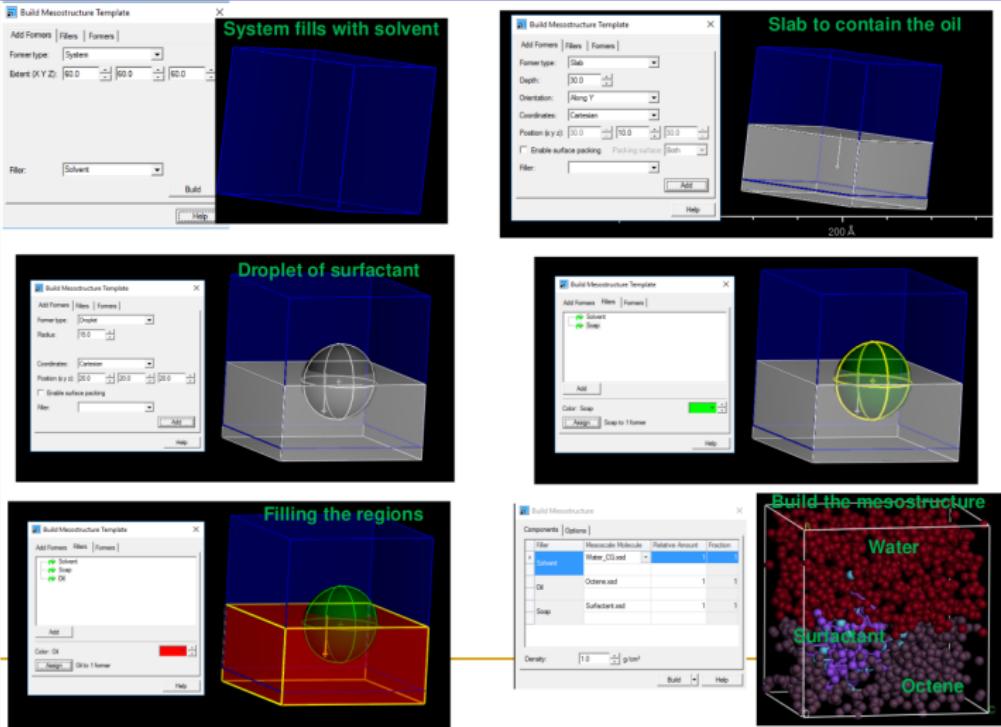


Fig.: Building Meso-molecule by temlapte for Materials studio.

MS Modelling: MOF Crystals

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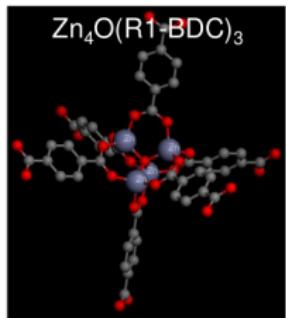
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Metal Framework Organic (MOF)
as prototypes of porous materials



Space Group : Fm(-3)m
Lattice : 25.8320 Å

Mohamed Eddaoudi et al. "Systematic Design of Pore Size and Functionality in Isoreticular MOFs and Their Application in Methane Storage", Science, 2002, 295, 469-472

	x	y	z	U(eq)
Zn	2934(1)	2066(1)	2066(1)	42(1)
O(1C)	2500	2500	2500	31(2)
O(1)	2819(2)	2181(2)	1340(2)	78(2)
C(1)	2500	2500	1113(3)	70(3)
C(2)	2500	2500	538(3)	75(3)
C(3)	2829(3)	2171(3)	269(3)	106(4)

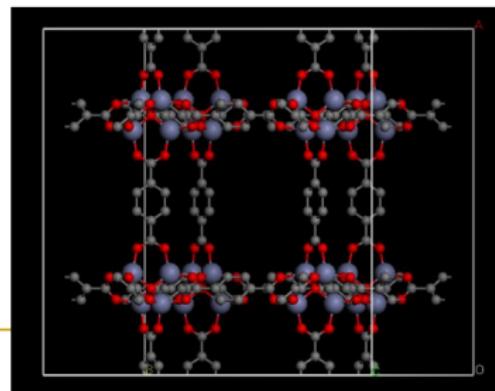
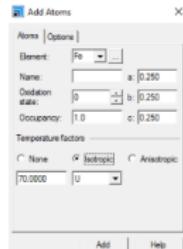


Fig.: Building Metal Framework Organic (MOF) for Materials studio.

MS Modelling: Miller Planes in Crystals



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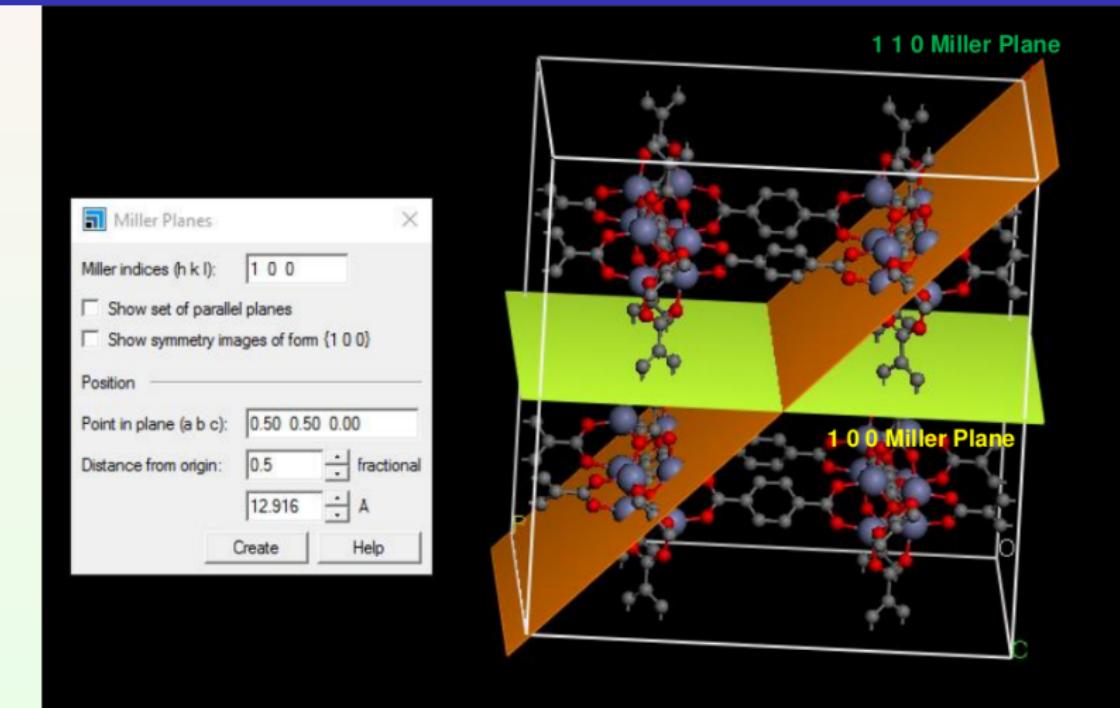


Fig.: Building Miller Planes in crystals for Materials studio.

MS Modelling: surface from Crystals

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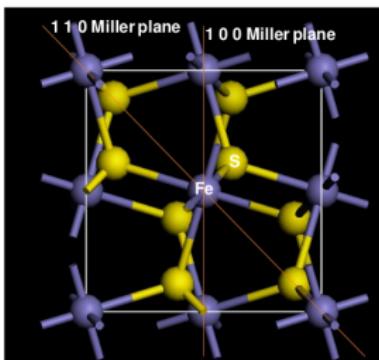
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1) Build the crystal

Space Group: Pa-3
Lattice Parameter: 5.417 Å
Fract. Coordinates: Fe (0,0,0)
S (0.3851, 0.3851, 0.3851)

Bayliss P, "Crystal structure refinement of a weakly anisotropic pyrite cubic model" American Mineralogist 62 (1977) 1168-1172



2) Cleave surface

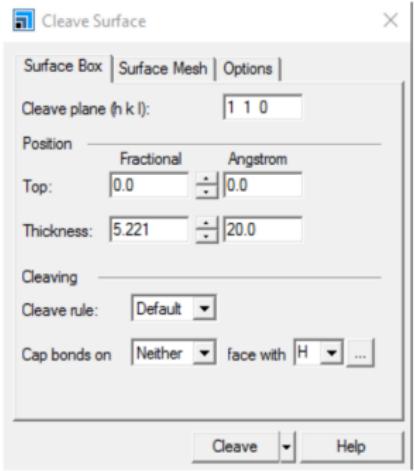


Fig.: Building surfaces from crystals for Materials studio.

MS Modelling: surface in Crystals

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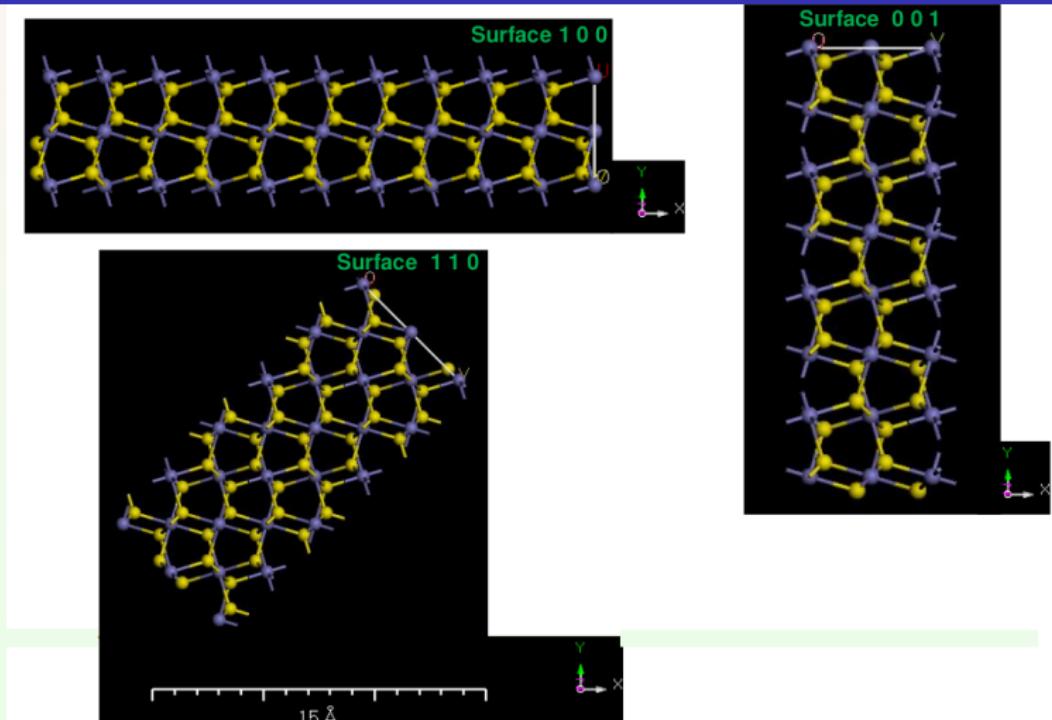


Fig.: Building surfaces in crystals for Materials studio.

MS Modelling: layers and vacuum

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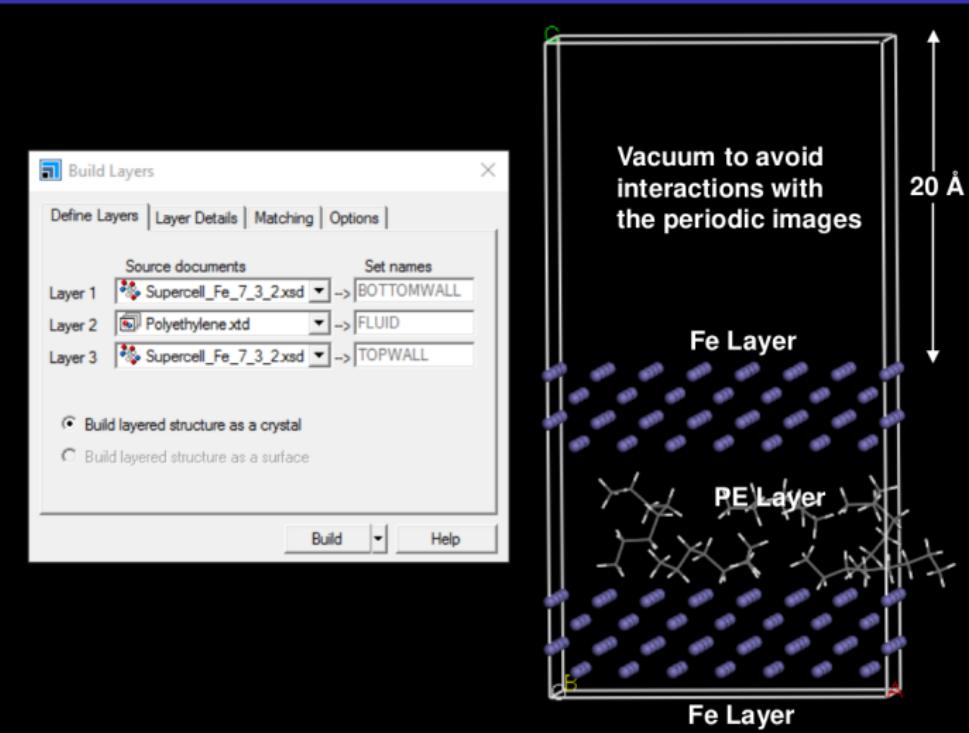


Fig.: Building metal-polymer-metal by multi-layers and vacuum for Materials studio.

Quantum simulation: Tools

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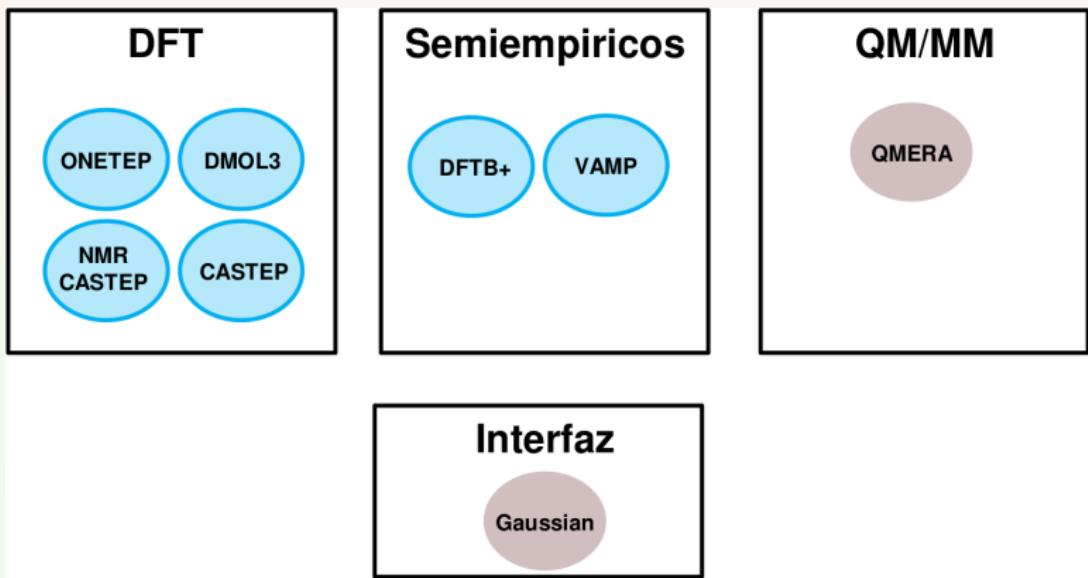


Fig.: Calculation modules for quantum simulation in Materials studio.

Ms Calculation modules comparison

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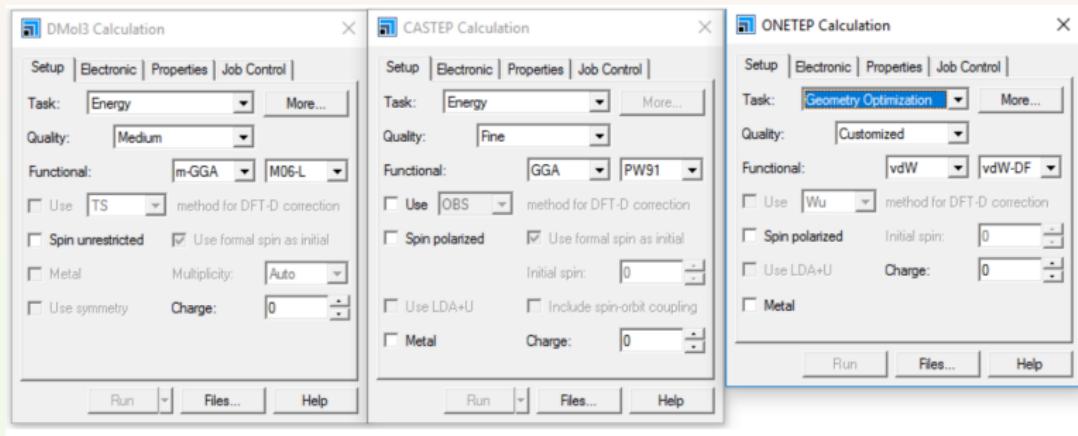


Fig.: Calculation parameters comparison in Materials studio.

Ms xc functional comparison

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Functional	DMOL3	CASTEP	ONETEP
LDA (Local Density Approximation)			
1980 VWN (Vosko-Wilk-Nusair)	X	X	
1981 CA-PZ (Ceperley-Alder-Perdew-Zunger)		X	X
1992 PWC (Perdew-Wang)	X		
GGA (Generalized Gradient Approximation)			
1988 BP (Becke-Perdew)	X		
1988 BLYP (Becke, Lee-Yang-Parr)	X		X
1992 PW91 (Perdew-Wang)	X	X	X
1992 VWN-BP (Vosko-Wilk-Nusair, Becke-Perdew)	X		
1996 PBE (Perdew-Burke-Ernzerhof)	X	X	X
1998 REV-PBE			X
1999 BOP	X		
1999 RPBE (Revised Perdew-Burke-Ernzerhof)	X	X	X
2001 HCTH	X		
2004 XLYP			X
2006 WC		X	X
2008 PBESOL	X	X	
Hybrids			
1993 B3LYP (Becke3, Lee-Yang-Par)	X	X	
1998 PBE0 (Perdew-Burke-Ernzerhof)	X		
2003 HSE03 (Heyd-Scuseria-Ernzerhof)	X		
2006 HSE06 (Heyd-Scuseria-Ernzerhof)	X		
Meta-GGA			
2006 M06-L Minnesota 2006 meta-GGA functional (Zhao-Truhlar)	X		
2011 M11-L Minnesota 2011 meta-GGA functional (Peverati-Truhlar)	X		
1994 M50 meta-GGA made simple, version 0	X		
1994 M51 meta-GGA made simple, version 1	X		
2003 TIPSS Tao, Perdew, Staroverov and Scuseria functional	X		
2009 revTIPSS revised Tao, Perdew, Staroverov and Scuseria funct.	X		
Non-local potentials			
HF (exact exchange, no correlation)	X		
HF-LDA (exact exchange, LDA correlation)	X		
sX (screened exchange, no correlation)	X		
sX-LDA (screened exchange, LDA correlation)	X		
VdW-DF (vdW from ab-initio, non-empirical corrections)			
2004,2010 vdW-DF (Dion, Roman)	X		
2010 vdW-DF2 (Lee)	X		
2010 optPBE (Klimeš)	X		
2010 optB88 (Klimeš)	X		
2010 Vdw-DFK (Klimeš)	X		

Dispersion corrections

Method for DFT-D correction	DMOL3	CASTEP	ONETEP
2009 TS Tkatchenko-Scheffler (PBE, BLYP y B3LYP)	X	X	
2006 Grimme (PBE, BLYP, B3LYP y TPSS)	X	X	
OBS (PW91 y LDA)	X	X	
1999 Moolj			X
2001 Elstner			X
2002 Wu			X

Fig.: XC functional comparison in Materials studio.

Ms Calculation modules comparison

Comparing DMol3, CASTEP and ONETEP

Tasks	DMOL3	CASTEP	ONETEP
Energy	X	X	X
Geometry optimization	X	X	X
Dynamics	X	X	X
Transition Structure Search	X	X	X
Transition Structure Optimization	X		
Transition Structure Confirmation	X	X	
Elastic Constants	X	X	
Reaction Kinetics	X		
Electron Transport	X		
Properties from other tasks		X	

Properties	DMOL3	CASTEP	ONETEP
Band structure	X	X	X
Density of states	X	X	X
Electron density	X	X	X
Electrostatics	X		X
Frequency	X		
Fukui function	X		
Optics	X		
Orbitals	X	X	X
Population analysis	X	X	X
Core level spectroscopy		X	
Electron localization function		X	

Fig.: Calculation modules comparison in Materials studio.

MS Calculation: ONETEP

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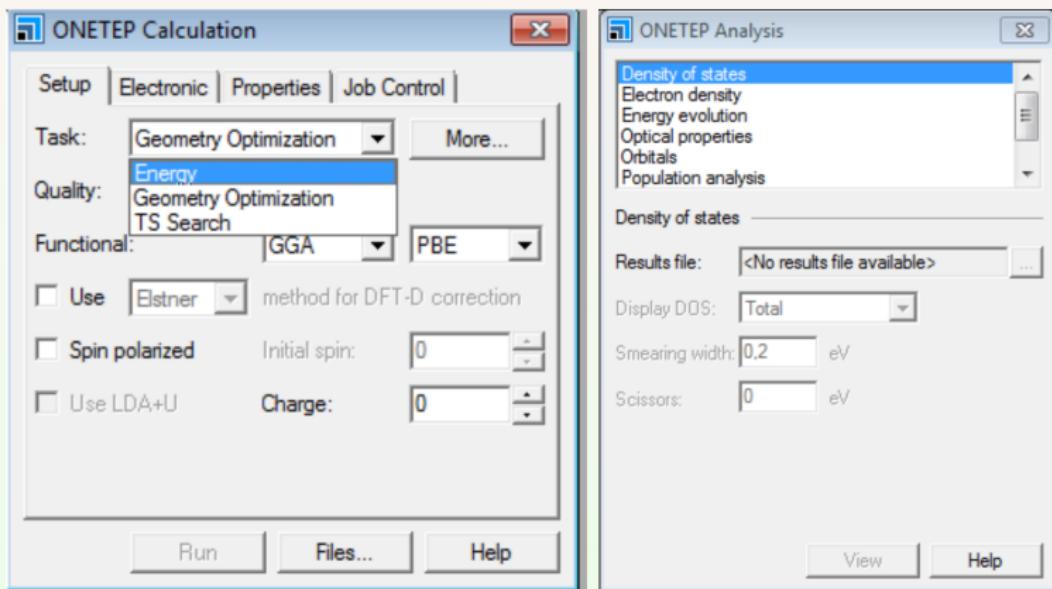


Fig.: Calculation module ONETEP in Materials studio.

MS Calculation: DFTB+ & VAMP

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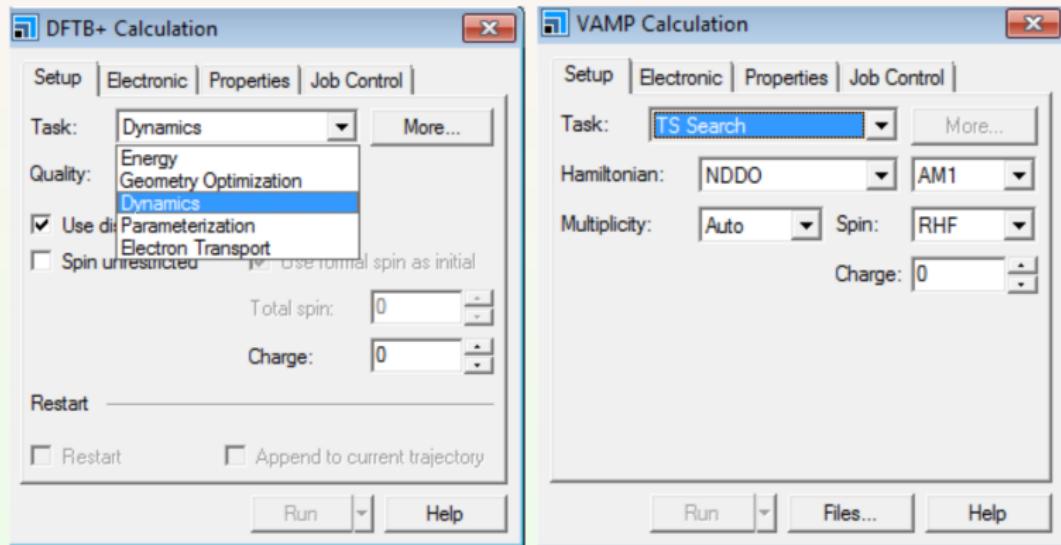


Fig.: Calculation parameters for module DFTB+ and VAMP in Materials studio.

MS Calculation: QMERA

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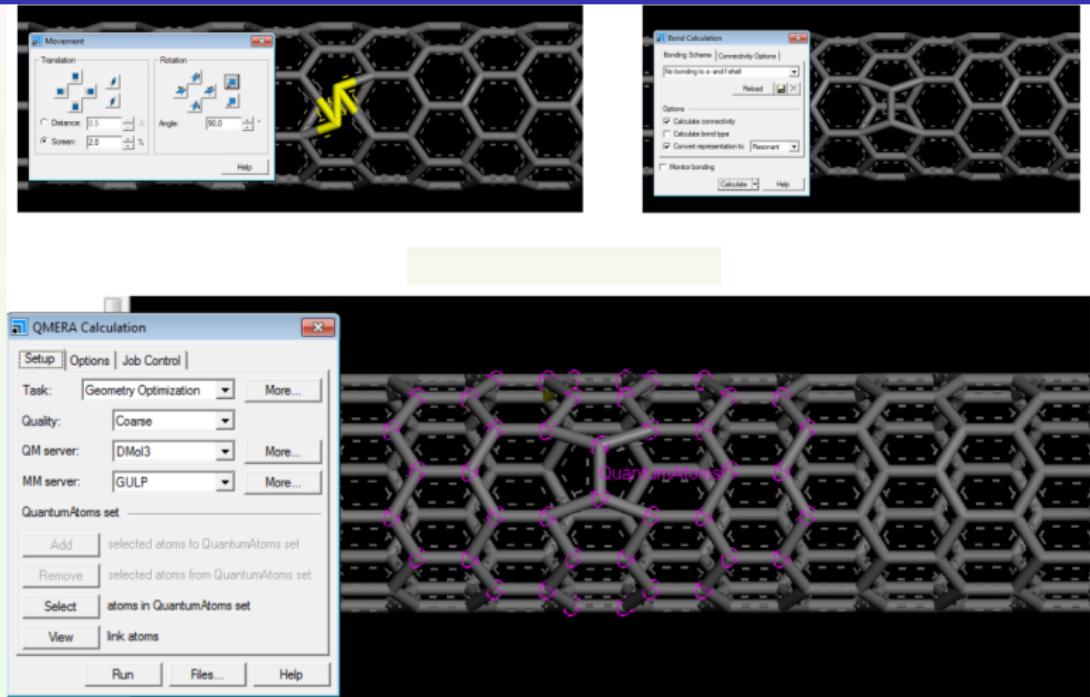


Fig.: Calculation parameters for module QMERA in Materials studio.

Classical simulation: Tools

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Molecular Mechanics (minimization) and Molecular Dynamics



Monte Carlo

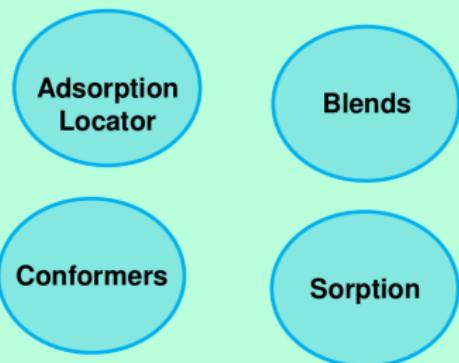


Fig.: Calculation modules for classical simulation in Materials studio.

MS Calculation: Forcite Plus

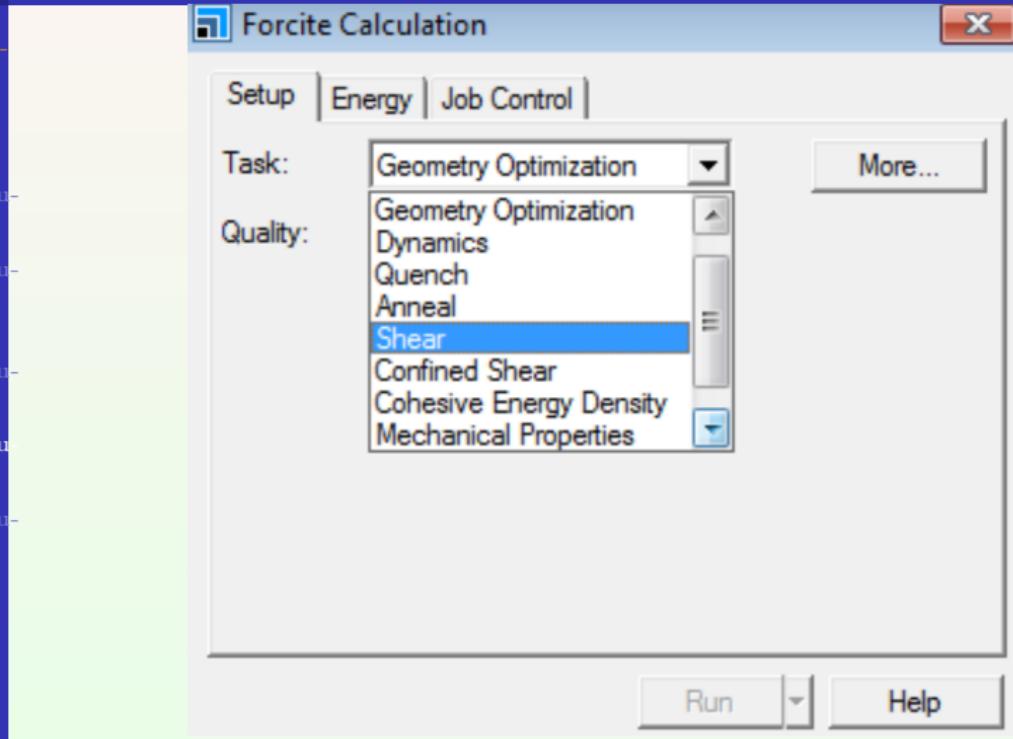


Fig.: Calculation modules Forcite in Materials studio.

MS Calculation: Adsorption Lactor

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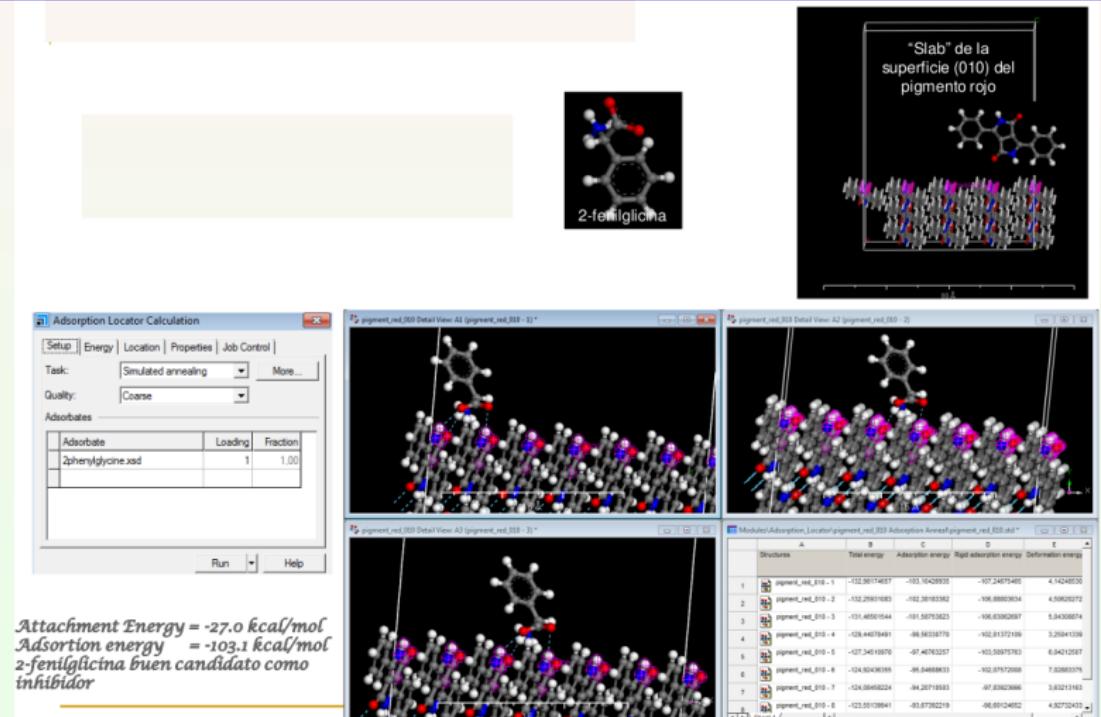


Fig.: Calculation modules Adsorption Lactor in Materials studio.

MS Calculation: Amorphous Cell

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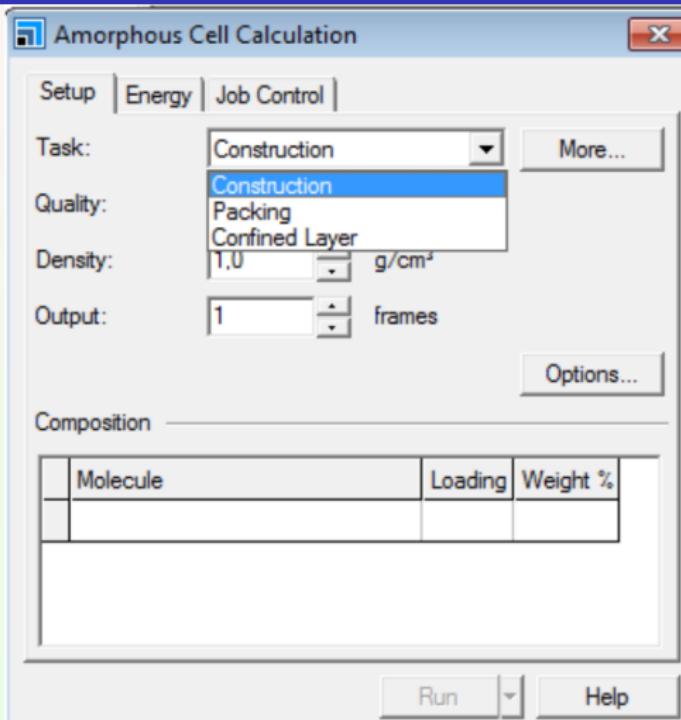


Fig.: Calculation modules Amorphous cell in Materials studio.

MS Calculation: Blends

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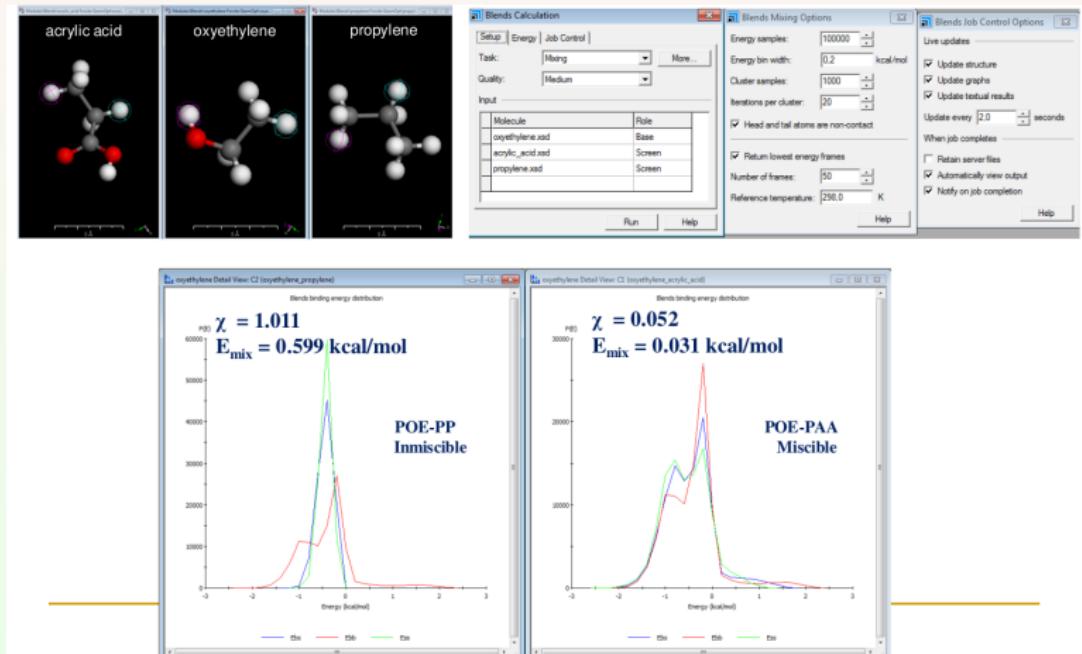


Fig.: Calculation modules Blends in Materials studio.

MS Calculation: Conformers

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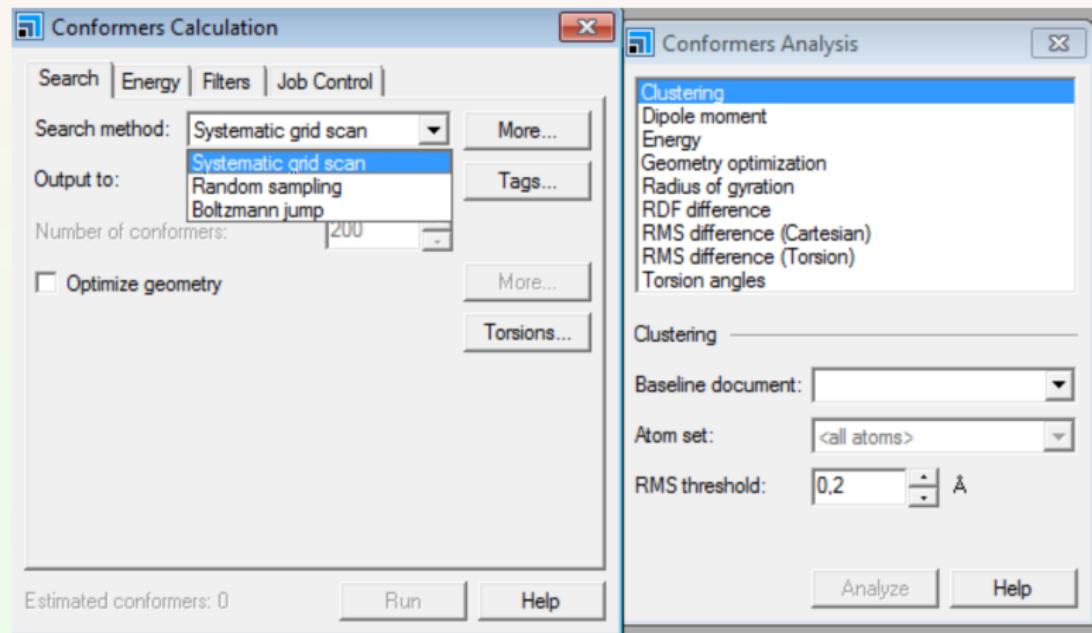


Fig.: Calculation modules Conformers in Materials studio.

Mesoescale simulation: Tools

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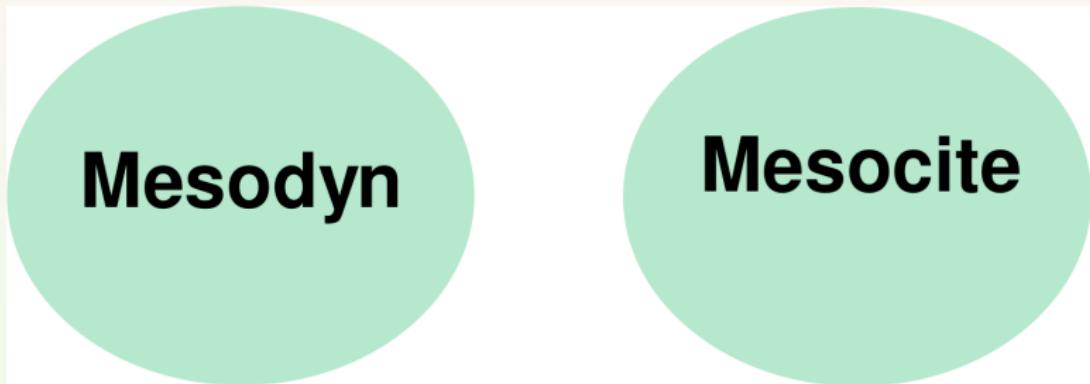


Fig.: Calculation modules for mesoscale simulation in Materials studio.

MS Calculation: Mesocite

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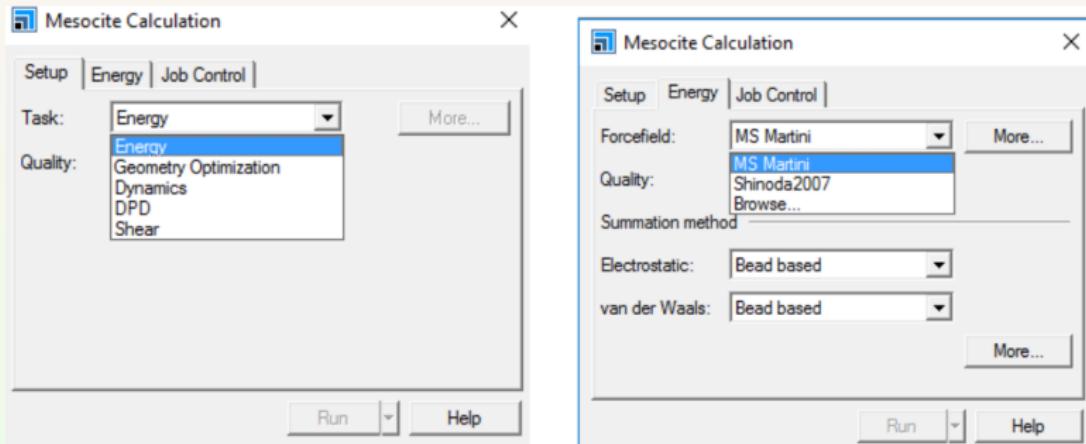


Fig.: Calculation modules Mesocite in Materials studio.

MS Analytical and crystallization tools

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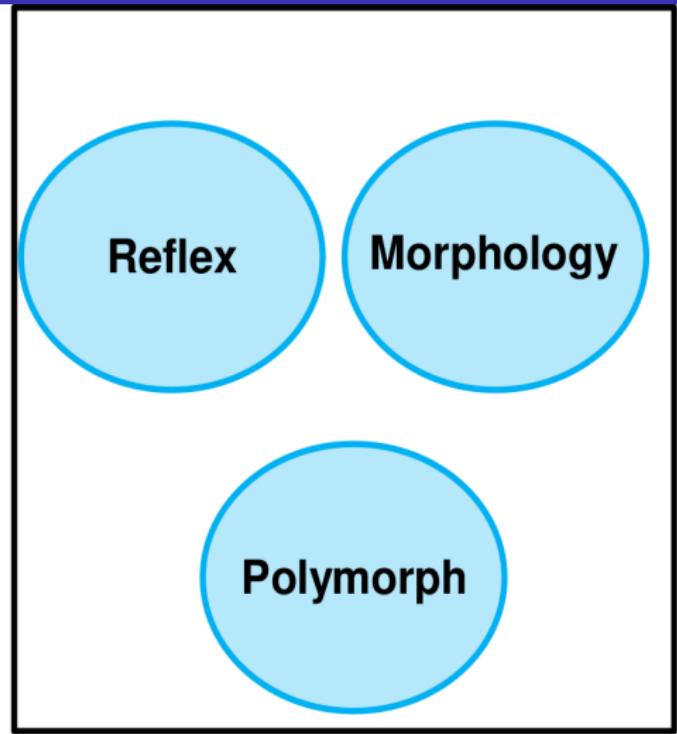


Fig.: Analytical and crystallization tools in Materials studio.

MS Analysis: Reflex

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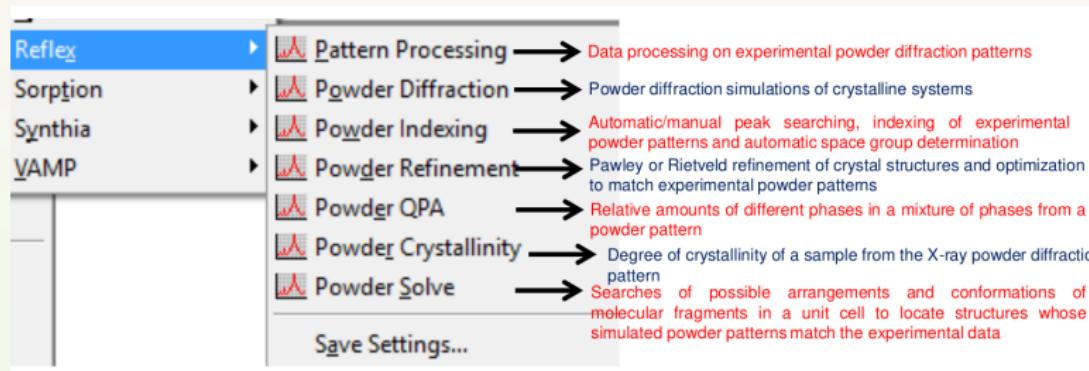


Fig.: Analysis module Reflex overview in Materials studio.

MS Analysis: Reflex

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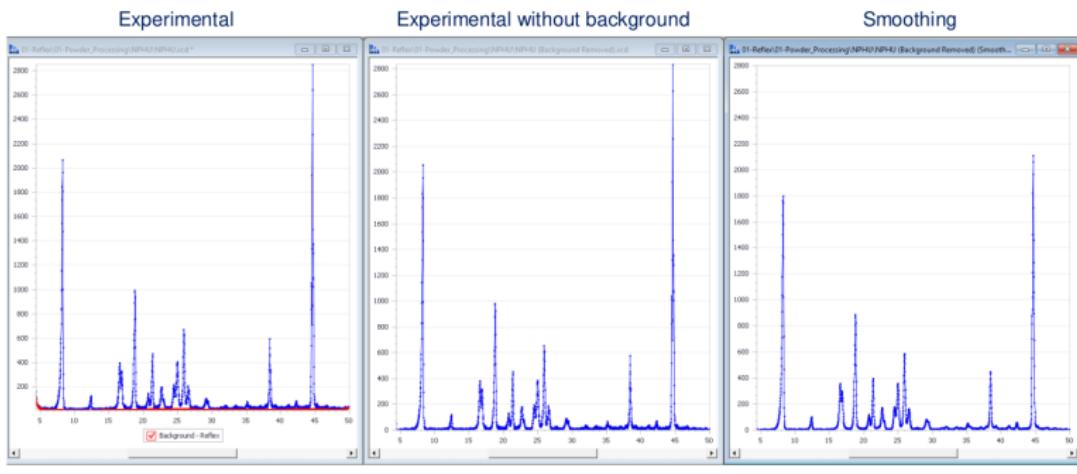
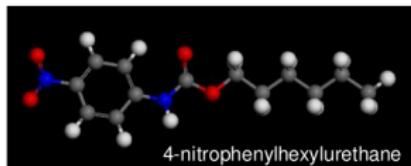


Fig.: Reflex pattern processing in Materials studio.

Reflex: Pattern Processing

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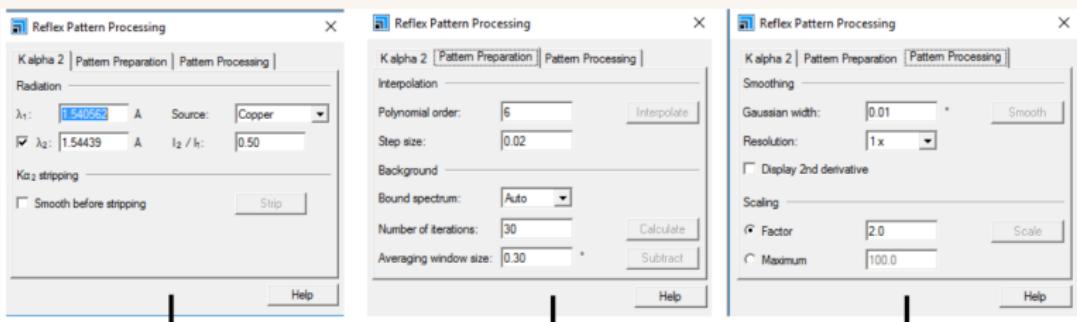
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Properties of the X-ray radiation used to obtain the experimental powder diffraction pattern and to strip K_{a2} peaks from a pattern

To perform interpolation and to calculate and remove the background scattering contribution from an experimental powder diffraction pattern

Data smoothing algorithm and scaling on an experimental powder diffraction pattern

Fig.: Pattern Processing parameters in Materials studio.

MS Analysis: Reflex

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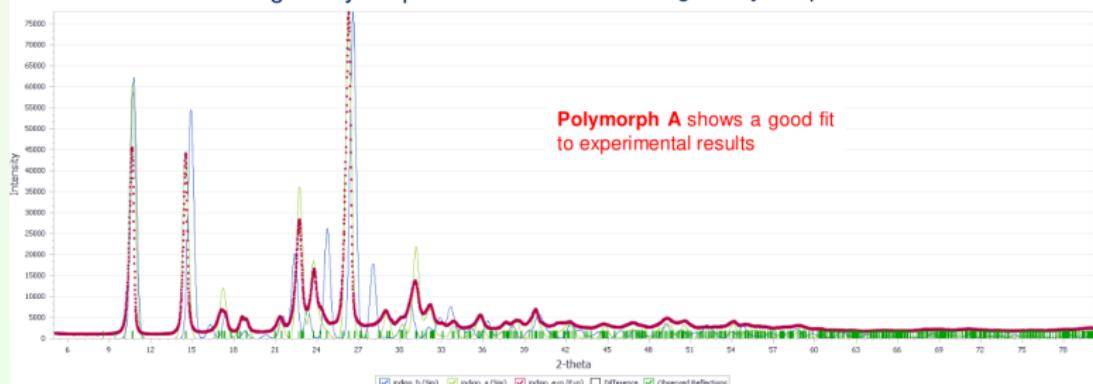
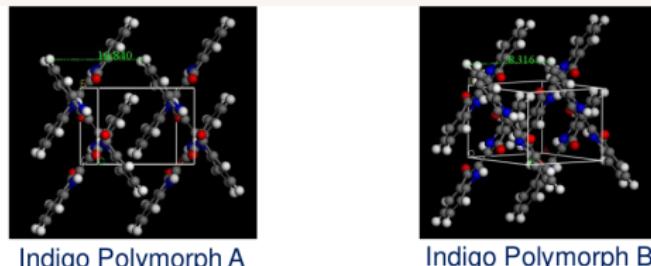


Fig.: Reflex powder diffraction in Materials studio.

Reflex: Powder Diffraction

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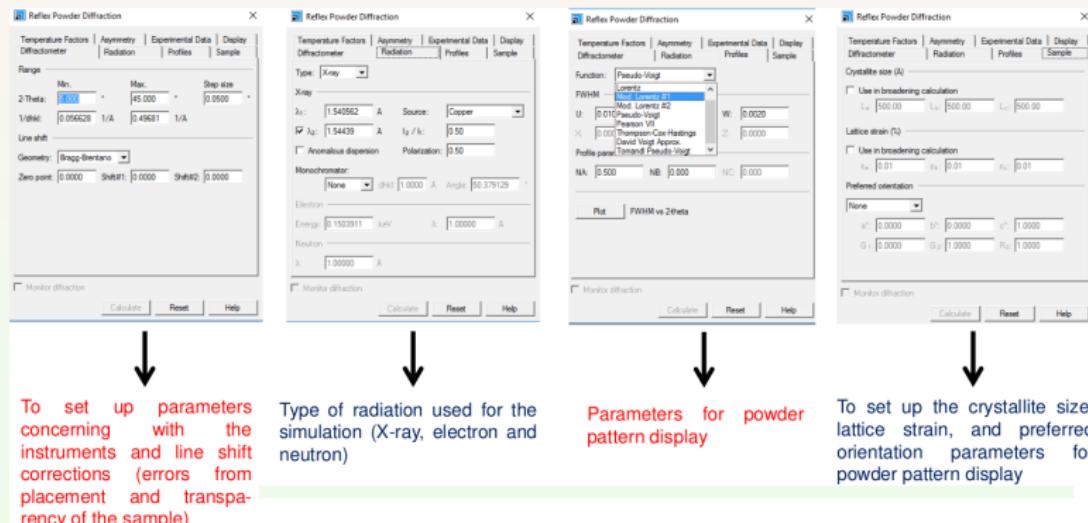


Fig.: Powder Diffraction parameters in Materials studio.

Reflex: Powder Diffraction

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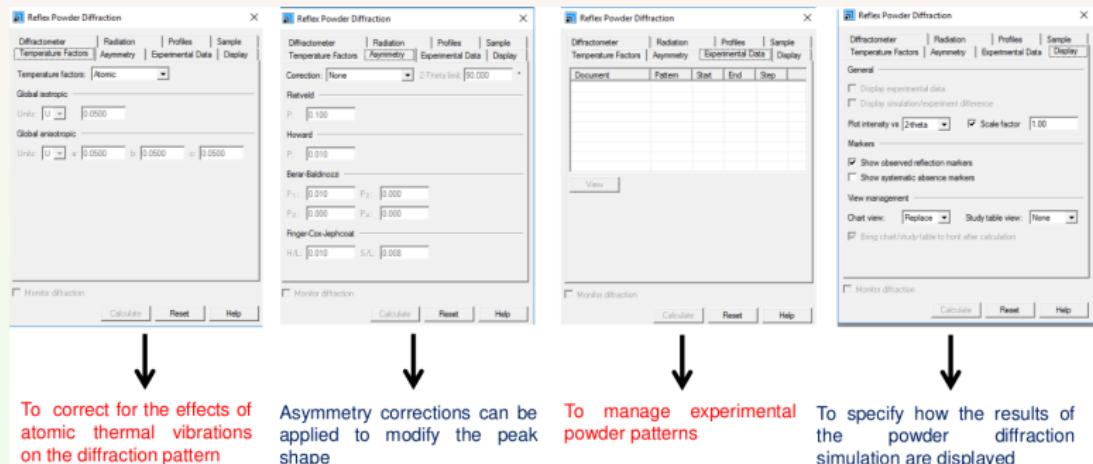


Fig.: Powder Diffraction parameters in Materials studio.

Reflex: Powder Indexing

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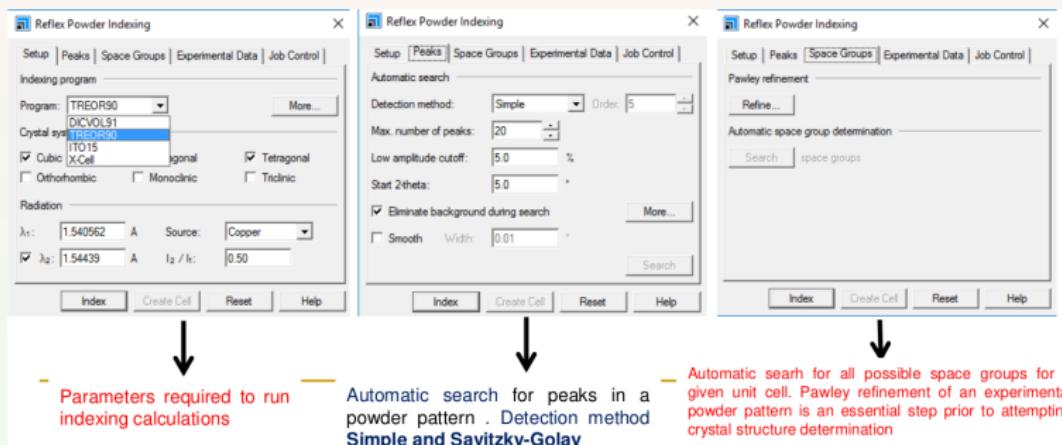


Fig.: Powder Indexing parameters in Materials studio.

Reflex: Powder Refinement

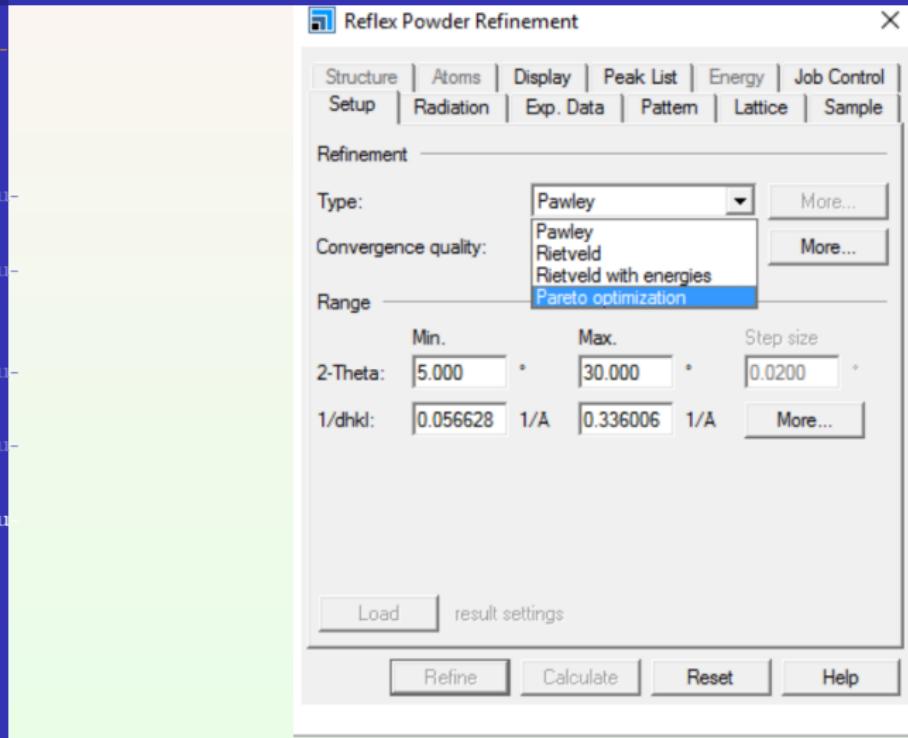


Fig.: Powder Refinement parameters in Materials studio.

Reflex: Powder QPA

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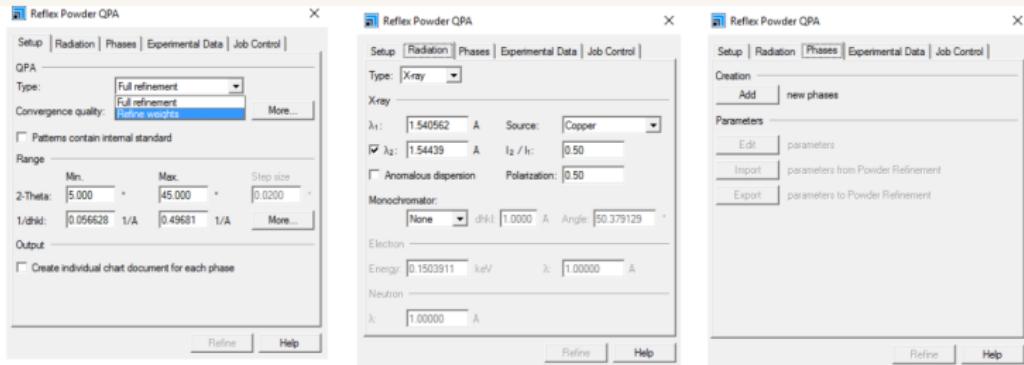
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- Type of refinement you wish to perform
- Modify the refinement control parameters
- Specify the range that will be used for the calculation of the measure of similarity between the simulated and experimental data
- Specify crystal structures or powder patterns for possible phases in the mixture
- Insert these documents into a study table for input to a Powder QPA calculation

Fig.: Powder QPA parameters in Materials studio.

MS Analysis: Morphology

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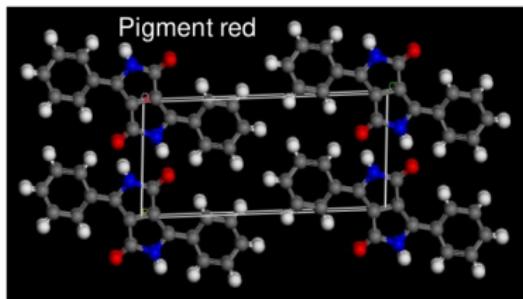
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➤ Geometry optimization of the crystal using FORCITE (COMPASS)



➤ Morphology Calculation → Growth Morphology using COMPASS force field

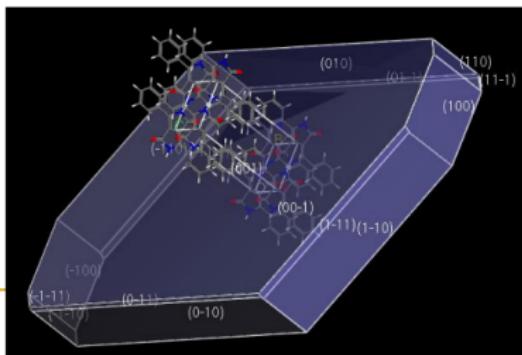


Fig.: Example: Morphology calculation in Materials studio.

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谢谢大家！