Using Materials Studio to Prepare and Run MD Simulations and Analyze the Results

Outline

- > Drawing an organic molecule using the sketch tool.
- Building a crystal structure (kaolinite, pyrophillite, talc, quartz...)
- > Cleaving the crystal along a certain crystallographic plane to create a surface
- > Optimizing crystal structure (geometry optimization or energy minimization)
- Creating a water box of 64 H₂O molecules and optimizing its structure
- Creating an aqueous solutions of (Na⁺, Cl⁻), or (Cs⁺, Cl⁻), (Ca²⁺, Cl⁻) or (Sr²⁺, Cl⁻) ... and using them to run MD and analyze the results
- Running MD Simulations
- Analyzing the MD results
- > Creating a slab of aqueous solution and adding it on the crystal surface
- > Running MD simulations for the interfacial clay-solution system and analyzing the results.

1. Drawing an organic molecule using the sketch tool

> Open Materials Studio.

> Choose 'create a new project' and name your project.

Welcome to Materials	Studio
num	Use the controls below to create a new project or open an existing one. Create a new project Open an existing project:
	D:\ngouana_VIRUS\Documents\Materials Studio Proj Browse
http://	Recent projects:
	D:\ngouancuments\Materials_Studio_Projects\Practicals.stp D:\ngouanDocuments\Materials_Studio Projects\Untitled.stp D:\ngouanuments\Materials_Studio Projects\Interfacial.stp D:\ngouants\Materials_Studio Projects\Montmorillonite.stp D:\ngouana_VIRUS\Documents\Materials_Studio Projects\NVT.stp C:\Users\uments\Materials_Studio Projects\Interfacial.stp D:\ngouana_VIRUS\Documents\Materials_Studio Projects\NPT.stp D:\ngouana_VIRUS\Documents\Materials_Studio Projects\NPT.stp D:\ngouan\Documents\Materials_Studio Projects\Dry-NPT.stp
	On start-up open the most recently used project
	OK Exit Aide

Right click on the name of your project -> New -> Folder Name it , e.g. 'NOM'

Now you can start sketching a model molecule of NOM (Natural Organic Matter) using the structure shown in the red frame of the file TNB-NOM-sein-est-1999-p1.pdf.

2. Creating a new MS project and building a crystal structure

- > Open Materials Studio.
- > Choose 'create a new project' and name your project.

Welcome to Materials	Studio
num	Use the controls below to create a new project or open an existing one. Create a new project Open an existing project:
http://	D:\ngouana_VIRUS\Documents\Materials Studio Proj Browse
	D:\ngouancuments\Materials Studio Projects\Practicals.stp D:\ngouanDocuments\Materials Studio Projects\Untitled.stp D:\ngouanuments\Materials Studio Projects\Unterfacial.stp D:\ngouants\Materials Studio Projects\Montmorillonite.stp D:\ngouana_VIRUS\Documents\Materials Studio Projects\NVT.stp C:\Users\uments\Materials Studio Projects\Interfacial.stp D:\ngouana_VIRUS\Documents\Materials Studio Projects\Interfacial.stp D:\ngouana_VIRUS\Documents\Materials Studio Projects\Interfacial.stp D:\ngouana_VIRUS\Documents\Materials Studio Projects\NPT.stp D:\ngouana_\Interfacials Studio Projects\Dry-NPT.stp
STUDIO	On start-up open the most recently used project OK Exit Aide

Right click on the name of your project -> New -> Folder Name it , e.g. 'crystal'

> Now you can start building the crystal or import (load) a template from a library.

2 (cont.). Building a crystal (kaolinite, pyrophillite, talc, quartz...)

You will be provided with unit cell atomic positions of some crystals. Choose one the structures and build the crystal.

Go to Build -> Crystals -> Build Crystal



Under Space group menu select the lowest symmetry group (P1), ignoring the symmetry group given by the atomic structure file. Then under Lattice Parameters enter the box lengths and angles.

Go to Build -> Add atoms

Add Atoms		×
Atoms Optic	ons	
Element:	0 💌	
Name:	0 x 0,0	00
Oxidation State:	0 • y: 0,0	od
Occupancy:	1,0 z: 0,0	00
Temperature F	actors	
None	C Isotropic C An	isotropic
	Add	Help

Input the coordinates for each atom to generate the crystal structure. Use the coordinates provided by the table "Co-ordinates for all atomic positions", but the identity of the atoms/elements (NoP) should be taken from the previous table in the same file.

3. Cleaving the crystal to create a surface

Go to Build -> Surfaces -> Cleave Surface

🖬 Cleave Surface 🗾 💌
Surface Box Surface Mesh Options
Cleave plane (h k l): 0 0 -1
Position
Top: -0.4589.591
Thickness: 0,976
Cleaving
Cleave rule: Default 💌
Cap bonds on Neither 🗸 face with H 💌
, , , , , , , , , , , , , , , , , , , ,
Cleave Help

Go to Build -> Crystal -> Build Vacuum Slab...

Ruild Vacuum Slab Crystal 🛛 🛛 💽				
Vacuum Slab Options				
Vacuum orientation:				
Vacuum thickness: 80,2418 Å				
Crystal thickness: 99,4785 Å				
Slab position: 0,00 Å				
Build Cancel Help				

- Define the cleavage plane (usually, it is (0 0 1))
- Define the thickness of the crystal

Cleave

- Choose the vacuum orientation
- Define the vacuum thickness (to be filled with aqueous solution later)



> Add hydroxils (OH groups) to the dangling bonds, if necessary

4. Creating a water box of 64 H₂O molecules

> Open Materials Studio.

> Choose 'create a new project' and name your project.

Welcome to Materials	Studio	×
num	Use the controls below to create a new project or open an existing one. Create a new project Open an existing project:	
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	On start-up open the most recently used project	
	OK Exit Aide	

Right click on the name of your project -> New -> Folder Name it 'Water'

> Now you can import (load) a template or build a model within the water folder.

Importing a template from the database



- Right click on the Water folder, then click on Import and go to /Structures/molecular-crystals/misc/ directory

- Chose the cubic ice structure (ice_cub.msi)

- Change space group to P1



You now have a unit cell with 8 water molecules (go to Edit -> Atom Selection menu to check for this). In order to make a simulation cell of 64 water molecules, you need to multiply the unit cell by (2 x 2 x 2) in the x, y, and z directions. - Create a supercell: Build -> Symmetry -> Supercell. Set supercell range to 2 for A, B and C and then click on supercell.

- You need now to resize the supercell dimensions to have them all equal. To do this you must calculate the volume needed to fit 64 water molecules in order to target a density of about 1 g/cm³. Find out this volume and from it, determine a, b, and c dimensions.

- Then, right click in the dark area -> Lattice Parameters -> Parameters. Now enter the a, b, and c values you just determined above.



- Make sure fractional coordinates are kept fixed while doing this.

Parameters Advance	:ed]			
Cell Origin (Å):	0,000	0,000	0,000	
Orientation standard:	C along 2	Z, B in YZ p	lane 💌	Re-orient to standard

Alternative method of creating a water box

- In the Water folder right click -> New -> 3D Atomistic Document. Rename it to water.xsd.
- Build a cubic crystal with a volume corresponding to 1 H₂O molecule: Build -> Crystals -> Build Crystal.

- As you did before, find out the volume needed to fit 1 H2O molecule if the density is equal to 1 g/cm^3 . From the volume deduce the box dimensions.

engths (Å)	-	Sec. 10. 10.		-21
a: 10,000	÷ b: 10,000	÷ c: [10,000	
ngles (degrees) at 90,000	β: 90,000	 	90,000	}
Sym	metry constraints: N	one		

- Select 1 P1 under Space group menu and enter the box dimensions you just determined under the Lattice Parameters menu.

- Then, Build -> Add Atoms -> Atoms.

Atoms Upti	ons	t
lement	U <u></u>	I
Name:	0	a: 0,000
Oxidation State:		b: 0,000
Occupancy:	1,0	c: 0,000
l'emperature f	Factors	
None	C Isotropic	C Anisotropic

- Choose Element O and enter the appropriate oxidation state. Set occupancy to 1,0, and atomic positions (a, b, c) so that the O atom is located at the center of the box.

- Click on the created O atom. Then Modify -> H Adjust Hydrogen

- You now have a box of $1 H_2O$ molecule.

Transform if into a box of 64 H₂O molecules.

5. Minimizing the crystal energy

(this part can be performed after connection to the license server)

- Go to Module -> Forcite tools. Click on the icon and then select Calculation.
 - > Select a task

Select the Forcefield

Set Computer options

Forcite Calculation	Forcite Calculation	Forcite Calculation
Setup Energy Job Control Task: Geometry Optimization V More Quality: Fine V	Setup Energy Job Control Forcefield: clayff More Charges: Forcefield assigned More Quality: Fine Summation method Electrostatic: Ewald Van der Waals: Ewald More	Setup Energy Job Control Gateway location: My Computer Queue: Job description: Automatic Run in parallel on: 2 1 of 4 cores
Run Help		Run Help

Click on More... to set options for the Task (where and if necessary)

- Run

6. Minimizing the energy (while connected to the license server)

- Go to Module -> Forcite tools. Click on the icon and then select Calculation.

> Choose a task

Choose the Forcefield

> Set Computer options

Forcite Calculation	Forcite Calculation	Forcite Calculation
Setup Energy Job Control Task: Geometry Optimization Quality: Fine	Setup Energy Job Control Forcefield: clayff More Charges: Forcefield assigned More Quality: Fine More Summation method Electrostatic: Ewald Image: More van der Waals: Ewald Image: More More	Setup Energy Job Control Gateway location: My Computer Image: Imag
	Run Help	More

Click on More... to set options for the Task (where and if necessary)

- Run	
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7. Creating aqueous solutions out of a pure water simulation box

- Create a new folder and a new 3D Atomistic Document in this folder. Then, open the minimized structure of water and copy paste it in your newly created 3D Atomistic Document.

- Select one O atom. Then go to Modify -> Modify Element -> Periodic Table and choose the element (Cs, Ca, Cl, Na, Li...) you want to replace with. Delete the two H atoms bonded to this new element.

- Repeat the procedure to add more elements of the same types.

- Remember that the elements you are adding are ions, double check that you have added an equal amount of positive and negative charge by your modifications in order to keep the total system neutral

- Minimize the energy of your system

8. Running MD Simulations (while connected to the license server)

- Go to Module -> Forcite tools. Click on the icon and then select Calculation.
 - Choose a task

Setup Er Task: Quality: Restart Restart	ergy Job Control	E d to cui	More
---	------------------	------------	------

Forcite Dynamics	—
Dynamics Thermo	stat Barostat Advanced
Ensemble:	NVT -
Initial velocities:	NVE NVT
Temperature:	NPH NPT K
Pressure:	0,0 GPa
Time step:	1,0 fs
Total simulation time:	5,0 ps
Number of steps:	5000
Frame output every:	5000 • steps
	Help

Forcite Dynamics	;	- ×-	Forcite Dynamic	:s	×	🔳 Forcite Dyna	mics	
Dynamics Thermo	ostat Barostat	Advanced	Dynamics Therm	nostat Barostat	Advanced	Dynamics T	hermostat Baros	tat Advar
nsemble:	NVT 💌		Ensemble:	NVT 💌	[]	Thermostat:	Berendser	•
tial velocities:	Random 💌		Initial velocities:	Random 💌	[Temp. differenc	e: Velocity So Nose	ale
nperature:	Random Current	к	Temperature:	298,0	к	Q ratio:	Andersen Berendsen	
ire:	0,0	GPa	Pressure:	0,0	GPa	Collision ratio:	NHL 1,0	
p:	1,0	fs	Time step:	1,0	fs	Decay constan	it: 0,1	рs
ulation time:	5,0	ps	Total simulation tim	. 5,0	ps			
of steps:	5000		Number of steps:	5000				
output every:	5000	steps	Frame output every	5000	steps			

🔳 Forcite Dy	mamics		- ×
Dynamics	Thermo	stat Barostat	Advanced
Ensemble:		NVT 💌	
Initial velocit	ies:	Random 💌	
Temperature	c	298,0	к
Pressure:		0,0	GPa
Time step:		1,0	fs
Total simulat	ion time:	5,0	ps
Number of st	eps:	5000 ÷	
Frame outpu	t every	5000	steps
			Help

Forcite D	ynamics		×
Dynamics	Thermo:	stat Barostat	Advanced
Thermostat		Berendsen	-
Temp. diffe	rence:	Velocity Scale Nose Andersen	
Q ratio:		Berendsen	
Collision rat	io:	1,0	
Decay con	stant:	0,1	ps
		[Help

These values can be 30, 30000, 100 for equilibration and 50, 50000, 4 after the restart to accumulate data for your equilibrium trajectory

Click on More... to set options for the Task

> Choose Forcefield, Set Computer options and Run

Forcite Calcula	ition	×
Setup Energy	Job Control	
Forcefield:	clayff 🗨	More
Charges:	Forcefield assigned	More
Quality:	Use current Charge using QEq	
Summation metho	Charge using Gasteiger Forcefield assigned	
Electrostatic:	Ewald 💌]
van der Waals:	Ewald 💌]
		More
	Run	Help

Setup Energy	on Job Control	
Gateway location:	My Computer	•
Queue: Job description:	 Au	<u>ت</u> utomatic
Run in parallel on:	2 in d cores	
		More

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9. Analyzing the results (while connected to the license server)

Sefore carrying out analysis, you need first to specify different groups of atoms in the system.

Go to Edit -> Atom Selection

Atom Selection	×
Select by Property:	Select All
Element	Deselect All
Is Cs	•
Selection mode	
Create a new selection from all	visible atoms
Select from the existing selection	n
Add to the existing selection	
Select	Help

Select the one atom or a group of atoms that will be used for analysis.

Go to Edit -> Edit Sets

Edit Sets	×
	New
	Delete
I	Select
	Help

Click on New and give a name to the set of atoms

📊 Define New Set		X
Name: Hydrogen		
🔽 Show set		
ОК	Cancel	Help

Repeat the previous steps to define other sets of atoms

Go to Module -> Forcite tools. Click on the icon and then select Analysis.

A list of properties is displayed on the left and their type (structural, dynamical, statistical) is given on the right.

Here we are going to look at the following properties:

Statistical properties Structural properties Dynamical properties Temperature Pressure **Radial distribution function** Mean squared displacement Hamiltonian (max distance – 10A) Velocity autocorrelation **Potential energy** \checkmark Concentration profile (think about the function and Power spectrum components directions: (0 0 1), (0 1 0), or (1 0 0); (use 3ps as the maximum length Total kinetic energy increase the number of bins to 500) of the VACF calculation) Forcite Analysis X Analysis / Category Anale distribution Structural Cell parameters Statistics Density Statistics Click on the property you want to analyze Density field Structural \geq Dipole autocorrelation function Dynamic Eluctuation propertie Dunamic Concentration profile Choose the sets of atoms (some properties require one set, some \geq Trajectory: water others – two) • Sets: 100 Specified direction (h k l) Choose or insert the appropriate options Number of bins Raw profile ÷ bins Smoothed profile Width: 3,0 Click on Analyze to launch the analysis \geq Frames to average Help Analyze

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