FROM ATOM TO POLYMER
CREATING AND MANIPULATING MODELS OF CHEMICAL COMPOUNDS IN BIOVIA MATERIALS STUDIO
What can be built in Materials Studio?

Single structures
What can be built in Materials Studio?

Homopolymers
What can be built in Materials Studio?

Block copolymers
What can be built in Materials Studio?
What can be built in Materials Studio?

Nanotubes
What can be built in Materials Studio?

Multi-wall nanotubes
What can be built in Materials Studio?

Nanopores
What can be built in Materials Studio?

Crystals
Getting started with Materials Studio

Save it as polymer
Getting started with Materials Studio

Import structure and modify

Sketch structure
Getting started with Materials Studio

[Image of a menu with the highlighted 'Import...' option]

Structures\repeat-units\imides\benzimid.msi
Getting started with Materials Studio
MS’s basic tools

MS provides wide spectrum of constructing system tools.

There are two basic panels:

- 3D Viewer
- Sketch

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- Selection
- Rotation
- Zoom
- Translation
- Reset view
- Recenter
- Fit to view
- Display style

- Sketch atom
- Sketch ring
- Sketch fragment
- Measure
- Create centroid
- Clean
- Adjust hydrogen
- Modify element
- Modify bond
- Modify hybridization
Getting started with Materials Studio

Click right button mouse on the background of 3D atomistic view
Getting started with Materials Studio

Select *Ball and stick* and set values *Stick radius = 0.1* and *Ball radius = 0.3*
Getting started with Materials Studio

Import structure and modify

Sketch structure
Getting started with Materials Studio

Select 3D Atomistic
Getting started with Materials Studio
Preparing the system

A key elements of preparation of simulations

- Geometric parameters of the system
  - Coords.
  - Atom types
  - Masses
  - Charges
  - Velocities

- Topologic parameters of the system
  - Bonds
  - Angles

- Interactions between atoms and molecules
  - Forcefield
MS’s basic tools

MS provides wide spectrum of constructing system tools.

There are two basic panels:

- **3D Viewer**
  - Selection
  - Rotation
  - Zoom
  - Translation
  - Reset view
  - Recenter
  - Fit to view
  - Display style

- **Sketch**
  - Sketch atom
  - Sketch ring
  - Sketch fragment
  - Measure
  - Create centroid
  - Clean
  - Adjust hydrogen
  - Modify element
  - Modify bond
  - Modify hybridization
Water – $\text{H}_2\text{O}$

Select **Sketch atom**, and change element to Oxygen from dropdown menu. Click anywhere on viewport.

Change element to Hydrogen and add two atoms in the close proximity.

Change **Display style** to **Balls and Sticks**.
Water – H₂O

By clicking on one of the atoms and dragging the line to another atom, the bond will be created.

Try to draw two bonds between oxygen and hydrogens.

Measure bonds lengths and angles using Mesure.
Water – H₂O

Now we will clean H₂O molecule.

Click Clean.

Molecule is initially optimized. Lengths and angle values are closer to real structure.

Angle: 104.45°
Bond: 0.95 Å
Biphenyle – $\text{C}_6\text{H}_{12}$

Create new 3D Atomistic document.

Biphenyle is a molecule containing two phenyl rings.

They can be constructed in two ways:

Use **Sketch fragment** to draw two phenyl rings and connect them,

Use **Sketch ring** to draw phenyl rings.
Biphenyl - C₆H₁₂

To draw proper structure of phenyl rings you have to add partial double bonds within aromatic ring. Hold ALT key using Sketch ring tool set partial double bonds between carbon atoms.

You can also select every bond in rings and change bond type by Modify bond type tool.
Biphenyle – $\text{C}_6\text{H}_{12}$

Now click **Adjust hydrogens**.

Missing hydrogens will appear.

Finally **Clean** your structure to obtain proper values of bonds lengths and angles.
Biphenyle – $\text{C}_6\text{H}_{12}$

Measure torsion angle between two phenyl rings using **Measure** tool. (~180°)

Click **View** | **Explorers** | **Properties explorer** to turn on **Properties** explorer.

Highlight value of torsion angle an check the value in Angle box.

Click twice on Angle and change it to 44 (which is experimental value).
Vitamin A - $C_{20}H_{30}O$

Build your own molecule – add atoms, change bonds, optimize structure.
Vitamin A - $\text{C}_{20}\text{H}_{30}\text{O}$
Polymers

- Homopolymers
- Random copolymers
- Block copolymers
- Dendrimers
How to create polymer?

Step-by-Step:

1. Building or importing molecule.
2. Modifying molecule.
4. Setting options of polymer.
5. Multiplying monomers.
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1. Building or importing molecule.

2. Modifying molecule.


4. Setting options of polymer.

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How to create polymer?

Step-by-Step:

1. Building or importing molecule.
2. Modifying molecule.
3. **Setting options of monomer.**
4. Setting options of polymer.
5. Multiplying monomers.
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Step-by-Step:

1. Building or importing molecule.
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How to create polymer?

Step-by-Step:
1. Building or importing molecule.
2. Modifying molecule.
4. Setting options of polymer.
5. **Multiplying monomers.**

Now let's go through all the points with graphical tutorial.
What do we want to get?
Building or importing molecules

Start new project and name it:

Poly-p-nitrostyrene
Building or importing molecules

Change Display Style to:
Ball and stick (SR = 0.1, BR = 0.3)
Modifying molecule

Choose Sketch fragment

Fragment Browser -> Functional Groups -> Nitro
Modifying molecule

Rename to: p-nitrostyrene
Setting options of monomer
Setting options of monome
Setting options of monomer

Click Head Atom
Setting options of monomer

Click Tail Atom
Setting options of monomer

Click Chiral Center
Setting options of homopolymer
Why atactic?
Why atactic?
Why atactic?

Atactic
Setting options of homopolymer
Multiplying monomers

Click build!
Multiplying monomers

Or you should get similar random structure of atactic homopolymer