



NTHRYS WORKSHOPS

Molecular Modelling For Materials Science

8:45 AM - 10:15 AM: Session 1: Modelling Polymers and Nanomaterials

Hands-on workshop on molecular modelling of polymers and nanomaterials. Protocols for building and simulating polymer structures and nanoparticles in different environments.

10:15 AM - 10:30 AM: Coffee / Tea / Snacks Break

Networking and refreshments.

10:30 AM - 12:00 PM: Session 2: Molecular Modelling of Crystals and Solid-State Materials

Practical session on modelling crystalline materials. Protocols for studying the properties and behaviors of solid-state materials at the molecular level.

12:00 PM - 1:00 PM: Lunch Break

Catered lunch and networking opportunity.

1:00 PM - 2:30 PM: Session 3: Modelling Molecular Interactions in Materials

Hands-on training on studying molecular interactions in materials.

Protocols for simulating van der Waals forces, hydrogen bonding, and electrostatic interactions in materials science.

2:30 PM - 2:45 PM: Short Break

Time for a stretch and informal discussions.

2:45 PM - 4:15 PM: Session 4: Predicting Material Properties Using Molecular Modelling

Practical session on predicting material properties.

Protocols for using molecular modelling to calculate mechanical, thermal, and electronic properties of materials.

4:15 PM - 4:30 PM: Coffee / Tea / Snacks Break

Last networking opportunity with snacks.

4:30 PM - 5:30 PM: Closing Session: Implementing Changes and Technology Adoption

Group discussions on implementing new techniques learned today.

Dialogue on overcoming challenges in adopting new technologies in similar sectors.

Feedback session and closing remarks.

Certificate Issue

5:30 PM: Workshop Concludes