



## NTHRYS WORKSHOPS

# Advanced Techniques In Molecular Dynamics

### 8:45 AM - 10:15 AM: Session 1: Advanced Simulation Methods

Introduction to advanced simulation methods in molecular dynamics.  
Hands-on session on using enhanced sampling techniques and coarse-grained simulations.  
Practical demonstration of advanced molecular dynamics simulations.

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

Networking and refreshments.

### 10:30 AM - 12:00 PM: Session 2: Integrating Molecular Dynamics with Experimental Data

Exploring approaches for integrating molecular dynamics with experimental data.  
Workshop on combining simulation data with X-ray crystallography, NMR, and other experimental techniques.  
Case studies on the benefits of integrative approaches in molecular dynamics.

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

Catered lunch and networking opportunity.

### **1:00 PM - 2:30 PM: Session 3: Multiscale Modeling**

Hands-on session on multiscale modeling techniques.  
Exploring techniques for bridging different scales in molecular dynamics simulations.  
Practical applications of multiscale modeling in complex systems.

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

Time for a stretch and informal discussions.

### **2:45 PM - 4:15 PM: Session 4: Computational Tools for Molecular Dynamics**

Workshop on computational tools and software for molecular dynamics.  
Practical techniques for using popular molecular dynamics packages.  
Case studies on the role of computational tools in enhancing molecular dynamics research.

### **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**