



Computational Chemistry Workshop

An Intensive and Interactive Onsite Short-Course for Scientists, Engineers, Technicians and Project Managers

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Day 1 Workshop Program/Synopsis...

- 8:30 AM** **Welcome, Introductions & Announcements**
- 9:00 AM Introduction to Computational Chemistry: Historical Perspective and Success Stories
- 9:30 AM Internet Resources for Computational Chemistry
- 10:00 AM **Morning Refreshment Break**
- 10:30 AM Review & Comparison of Commercial Modeling Software
- 11:30 AM Theory and Applications of Molecular Mechanics - I: Classical Force Fields
- 12:00 Noon** **Non-Host Group Luncheon (catered)**
- 1:00 PM Theory and Applications of Molecular Mechanics - II: More About Classical Force Fields
- 2:00 PM **Demos & Supervised Hands-On Exercises:**
Build your own molecules!
- 2:30 PM **Afternoon Refreshment Break**
- 3:00 PM Geometry Optimization of Molecules
- 4:00 PM **Demos & Supervised Hands-On Exercises:**
Optimization of your molecular systems
- 5:00 PM Day-1 Adjournment

Day 2 Workshop Program...

- 9:00 AM Review of Day-1 Highlights - Questions?
- 9:30 AM Review of Basic Quantum Mechanics (Molecular Orbital) Theory
- 10:30 AM **Morning Refreshment Break (Well deserved after QM review!)**
- 11:00 AM QM Calculation Methods: Semiempirical, *Ab Initio* and Density Functional
- 12:00 Noon** **Non-Host Group Luncheon (catered)**
- 1:00 PM **Demos & Supervised Hands-On Exercises:**
How to set up and carry out QM calculations...
- 2:00 PM Computer-Aided Drug Discovery (CADD) - **Guest Speaker**
- 3:00 PM **Afternoon Refreshment Break**
- 3:30 PM **Demos & Supervised Hands-On Exercises:**
Building and optimizing more complex systems...
- 5:00 PM Day-2 Adjournment

Day 3 Workshop Program...

- 9:00 AM Review of Day-1&2 Highlights - Questions?
- 9:30 AM Molecular Dynamics (MD) Simulations - Theory

- 10:30 AM **Morning Refreshment Break (Well deserved after MD review!)**
- 11:00 AM Monte Carlo and Langevin Dynamics
- 11:30 AM Molecular Dynamics in Practice - Periodic Boundaries, Ensembles, etc.
- 12:00 Noon **Non-Host Group Luncheon (catered)**
- 1:00 PM **Demos & Supervised Hands-On Exercises:**
How to set up and carry out an MD (or MC) simulation...
- 2:30 PM **Afternoon Refreshment Break**
- 3:00 PM Extracting Useful Information from MD Simulations: **More Demos...**
- 4:00 PM Review and Q&A Session - Open Discussion
- 5:00 PM **Workshop Adjournment**
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