

A Brief Introduction to Gaussian
Umea, Sweden
May 14 – May 15, 2018



Day 1: Monday, May 14

- 8:45** Check In & Distribution of Workshop Materials
- 9:00** Chemical Potential Energy Surface Review
- Designing Computational Experiments
 - Potential Energy Surfaces
 - Optimizing Reactants & Products
 - Optimizing Transition States & Reaction Path Following
 - Vibrational Spectroscopy & Thermochemistry
- 10:30** Tea & Coffee Break
- 10:45** Laboratory I: Chemical Exploration
- 12:00** Lunch
- 13:00** Model Chemistry Review
- Basis Sets
 - Density Functional Theory
 - Semi-Empirical & Molecular Mechanics Theories
 - ONIOM Hybrid Methods
- 14:45** Tea & Coffee Break
- 15:00** Laboratory II: ONIOM Adventures
- 17:00** Departure

Day 2: Tuesday, May 15

- 9:00** Solutions & Spectroscopies
- Self-Consistent Field Problems & Strategies
 - Solvation Models
 - TD-DFT & UV Spectroscopy
- 10:45** Tea & Coffee Break
- 11:00** Laboratory III: Solution-phase Chemistry
- 12:00** Lunch
- 13:00** Laboratory IV: Excited States
- 14:45** Tea & Coffee Break
- 15:00** Laboratory V: Open-shell & Paramagnetic Systems
- 17:00** Departure