

Computational Chemistry/Materials Tutorial, sponsored by CEI

Instructor:

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Time:

Tuesdays	1:00pm - 2:00pm	Lecture (Zoom)
	2:00pm - 4:00pm	Tutorial Session (Zoom)

Course Description: This is a tutorial style course, so obviously there are no tests or grades assigned. The main purpose of this tutorial course is to give an overview of computational chemistry and computational materials, how to run Gaussian/VASP jobs, and build molecular systems using GaussView/VESTA. Starting from the 4th week, students will choose two different study tracks - computational spectroscopy using Gaussian and computational materials using VASP. Students taking this course will be split up into smaller groups of ~ 10 people or less for the tutorial sessions. Tutorials will start with basic computational jobs using Gaussian or VASP, and will be tailored to the need of each tutorial groups.

Getting Started: Instructions for using Gaussian, Gaussview, VASP, and VESTA are located in the “**Software and Installation Instructions**” document, but will be covered in the first tutorial.

Tentative Course Outline:

The weekly coverage might change as it depends on the what people may want to focus on. Additionally, after the first few sessions tutorial groups will diverge in content based on their needs.

Week	Lecture	Computer Lab
Week 1	From Wave Function to Computational Chemistry/Materials	<ul style="list-style-type: none"> • Setting up GaussView • Mox accounts, Gaussian access. • Submit Gaussian Jobs
Week 2	Geometry and Wave Function Optimizations	<ul style="list-style-type: none"> • Molecular geometry optimization • Transition states • Reaction pathways
Week 3	Density Functional Theory and Electron Correlation	<ul style="list-style-type: none"> • Orbital visualization • Property analysis • Solvation models
Week 4	Track #1: Computational Spectroscopy using Gaussian	<ul style="list-style-type: none"> • UV-Vis spectroscopy • IR/Raman spectroscopy
	Track #2: Computational Materials using VASP	<ul style="list-style-type: none"> • Crystal structures • Periodic boundary conditions
Week 5	Track #1: Computational Spectroscopy using Gaussian	<ul style="list-style-type: none"> • X-ray absorption • Emission
	Track #2: Computational Materials using VASP	<ul style="list-style-type: none"> • K-point sampling • Band structures
Week 6 and Beyond	Special Topics	<ul style="list-style-type: none"> • Special topics