CHEM-365 : Computational Chemistry

Designed to introduce students to the fundamental principles and techniques of computational chemistry. Approaches to be discussed include molecular mechanics, molecular dynamics, and density functional theory, among others. Discussion will focus on supporting, not replacing, the work of traditional synthetic chemists, and particular attention will be paid to the strengths/limitations of each technique for one or more specific purposes. Students will learn to model molecular systems and to critically analyze a potential energy surface, identifying local and global minima and the transition states between them. The application of these tools in ligand design and drug discovery will be a key component. Offered alternate years.
Credits 3
Prerequisites
CHEM-306 or CHEM-310
Term Offered
Spring Only
Session Cycle
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