Molecular modeling and Chemical Information (CHEM 3301) **Fall 2024**

Class time: 9:00 am – 11:50 am, CCSB 1.0204

Course Description

CHEM 3301, Molecular Modeling and Chemical Information, is an upper division course that provides introduction to computational chemistry methods for molecular electronic structure, energy, geometry optimization, and reactivity, includes strategies for chemical data analysis, and obtaining chemical information from electronic sources. The basic tools of quantum chemistry, computational chemistry and theoretical chemistry are acquired through this course. The technical skills acquired in the course are essential to and serve as the basis for professions related to molecular simulations and drug design, this includes the confident use of the Gaussian quantum chemistry program package, GaussView6 visualizer and HPC of UTEP. Understanding the workflow of scientific computing and hands-on knowledge about quantum chemical calculations will be learned as well.

Learning Objectives

The general aim of the course is putting several key concepts of physical, analytical and inorganic chemistry, including wavefunction, molecular geometry, absorption/emission in the IR and UV-Vis region, pKa, reduction potential, dative bond, etc. into a molecular perspective through quantum chemical calculations on simple systems. Managing high-performance computers, using a leading quantum chemistry software (Gaussian16) and an all-purpose visualizer and molecular editor (GaussView6), obtaining chemical information and organization of data are the fundamental skills that will be mastered through this course. A part of the course will also provide introduction to python programming for analysis of chemistry-related datasets and training predictive machine learning models on those datasets. The program of the course is designed to promote individual thinking, work, and time management, helping students to prepare for their professional careers.

Required

1. Laptop with MS Windows (UTEP Technology Support can lend it for the semester if needed):
2. Internet connection
3. Software: MS Word and Excel, Notepad++, ChemDraw, Mercury, GaussView, Gaussian Utilities, Bitvise, Putty, WinSCP, Global VPN/Duo Mobile, Vim, Google Colab (for python notebooks)

Summary of Classes and Reports

[1] Class 1. – Introduction. Introduction to the requirements of the course. Introduction to computational chemistry methods, density functional theory and high performance computing. Finishing Installation necessary softwares. Learning the protocol to communicate with the HPC center, basic commands of Linux. Introduction of Gaussview6. (no report due for class 1 / week 1)

[2] Class 2. – Energy - SCF. Introduction of Self-consistent-field iterative protocol, functionals and basis sets of DFT. Calculation of molecular energy with different density functional theory methods and monitoring the convergence of the Self-Consistent Field iterative protocol. The dependence of molecular energy on the DFT functional and basis set is investigated. Learning to confidently use one of the leading quantum chemical codes, Gaussian16. Writing input files, analyzing output files, extracting useful information from the calculations, like atomic charges, molecular structure, and energy.

[3] Class 3. – PES – Equilibrium structure Geometry optimization to compute the molecular equilibrium structure of simple molecules, including H2O, CH4, CO2 , O3 and NH3. Using visualization programs to create the initial structure, monitoring the geometry convergence and to analyze the optimized geometry. Analysis of the equilibrium structure, comparison to experimental structure.

[4] Class 4. – Covalent Bonds and Molecular Orbitals internuclear potential of homoatomic diatomics. Calculation of the molecular energy of diatomics at different bond lengths and construction of the internuclear potential. Comparison to Morse, Lennard-Jones and quadratic potentials and BDE estimation. Analysis of the electronic structure of simple molecules using molecular orbitals and atomic charges. Determining the strength of dative

bonds in Lewis pairs and its dependence on substituents and correlated with bond order measures. Interpretation of dative bond within MO theory.

[5]. Class 5. – Vibrations and Frequency calculations. Running frequency calculations and analysis of results; visualizing and determining the symmetry and energy of vibrations. Comparison of calculated data with experimental data obtained from IR spectroscopy.

[6] Class 6. – Relative stability & thermochemistry in DFT. Determining the relative stability of isomers. Thermal contributions to the electronic energy will be discussed. Application of thermochemistry and the calculation of enthalpy, free energy and Gibbs free energy will be demonstrated.

[7] Class 7. – pKa calculations. Calculation of the pKa of simple organics using multiple methods Implicit solvation is introduced.

[8] Chemical phenomenon 8. – Reduction potential. Calculation of the reduction potential of a metal and a ligand centered electron transfer in Ru(bpy)3-type and organic systems using the Born-Haber thermodynamic cycle.

[9] Class 9. – Programming and work with large datasets. Students will gain an in-depth understanding of handling and processing large datasets using Python. We will explore best practices, tools, and techniques that make it easier and efficient to work, visualize and explore large data sets

[10] Class 10. – Machine learning I. Foundational introduction to machine learning using Python. We'll demystify what machine learning is and how it works, and provide students with a solid understanding of its principles, algorithms, and applications.

[11] Class 11. – Machine learning II. This class offers a unique blend of computational chemistry and modern data science, wherein students will leverage Density Functional Theory (DFT) calculations to create a dataset, and then harness machine learning techniques for predictive modeling.

Reports instructions

Reports summarize the findings of activities. The reports associated with quantum calculations contain six sections: 1. Aim of the activity, 2. Methodology (provided in a way that the results can be reproduced), 3. Investigated molecules, 4. Name and location of output files used to write the report, 5. Results, 6. Conclusions. They are written in MS Word and figures must be created with ChemDraw, Excel.

Instructions on the reports on python programming and machine learning and their sections will be provided with the assignments.

Reports due on Fridays at 10:00 pm on the week following the class. (Delayed reports: minus 20 points/week)

Grading

The final grade is based on a points system: 10 reports with 100 pts each, making a total of 1000 points.

Final Grade	Points	% Required
A	900-1000	90%-100%
B	800-899	80%-89%
C	700-799	70%-79%
D	600-699	60%-69%
F	<599	<59%

Week	**Experiment**
August 30	Class 1. – Introduction
September 6	Class 2. – Energy – SCF.
September 13	Class 3. – Equilibrium structure
September 20	Class 4. – Covalent bonds and Molecular orbitals

September 27 Class 5. – Vibrations and Frequency calculations
October 4 Class 6. – Relative stability & thermochemistry in DFT
October 11 Class 7. – pKa calculations
October 18 Class 8. – Reduction potentials
October 25 Class 9. – Programming and work with large datasets
November 1 Assistance with issues (python examples, if needed)
November 8 Class 9. – Machine learning I.
November 15 Class 10. – Machine learning II.

Accommodations policy

The University is committed to providing reasonable accommodations and auxiliary services to students, staff, faculty, job applicants, applicants for admissions, and other beneficiaries of University programs, services and activities with documented disabilities in order to provide them with equal opportunities to participate in programs, services, and activities in compliance with sections 503 and 504 of the Rehabilitation Act of 1973, as amended, and the Americans with Disabilities Act (ADA) of 1990 and the Americans with Disabilities Act Amendments Act (ADAAA) of 2008. Reasonable accommodations will be made unless it is determined that doing so would cause undue hardship on the University. Students requesting an accommodation based on a disability must register with the UTEP Center for Accommodations and Support Services (CASS). Contact the Center for Accommodations and Support Services at 915-747-5148, email them at cass@utep.edu, or apply for accommodations online via the CASS portal.

COVID-19 PRECAUTIONS

Please stay home if you have been diagnosed with COVID-19 or are experiencing COVID-19 symptoms. If you are feeling unwell, please let me know as soon as possible, so that we can work on appropriate accommodation. If you have tested positive for COVID-19, you are encouraged to report your results to covidaction@utep.edu. For more information on COVID-19 testing at UTEP, please visit: https://www.utep.edu/ehs/covid/.