CLARK ATLANTA UNIVERSITY
SCHOOL OF ARTS AND SCIENCES

DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS

COURSE PREFIX, NUMBER & TITLE: CHE 4XX & COMPUTATIONAL CHEMISTRY AND MOLECULAR MODELING

CRN	Semester Hours	Course Section	Meeting Days	Meeting Time	Meeting Location	Level *(U/G)*
???	4	01	T R T	1:30 – 3:00 pm 3:15 – 6:00 pm (Lab)	Remote via Zoom Remote via Zoom	U

Instructor _Dr. Dinadayalane Tandabany (**Dr. Dina**), Associate Professor_____

Office Hours	
Office Location	
Office Telephone	(404)-880-6969
Email	dtandabany@cau.edu

Course Description:

This 4-credit course is the lecture and lab to introduce the concepts of computational chemistry and molecular modeling and their applications in chemistry and biology. This course is mainly for upper level undergraduate students of chemistry and biology majors but students in any STEM discipline can take this course. Computational chemistry and molecular modeling is a rapidly developing discipline and has benefited from the dramatic improvements in computer hardware and software in recent years. Today's computer workstations are very powerful. Scientific software can be obtained from commercial software companies and academic laboratories. Thus, molecular modeling can be performed in any laboratory or classroom. The main purpose of this course is to introduce some of the techniques used in computational chemistry and molecular modeling and to demonstrate how these techniques can be used to study physical, chemical and biological phenomena. Computational chemistry and molecular modeling studies involve three stages. In a first stage, a model is selected to describe the intra- and inter-molecular interactions in the system. The most common models that are used in molecular modeling are quantum mechanics and molecular mechanics. These models enable the energy of any arrangement of the atoms and molecules in the system to be calculated, and allow the modeler to determine how the energy of the system varies as the positions of the atoms and molecules change. The second stage is the calculation itself, such as an energy minimization, single-point energy calculations, and conformational search. In the final stage, the calculation must be analyzed, not only to calculate properties but also to check that it has been performed properly. The students in this course will learn different stages of molecular modeling studies mentioned above and applications of computers in chemistry as well as related fields like molecular sciences, drug design, biomedical, and materials science. This course is intended to prepare undergraduate students for higher education on computational-based research in chemistry, biology or engineering by introducing the concepts and techniques used in computational chemistry and molecular modeling.

Prerequisites (*if applicable)*:

General Chemistry I and II (CHE 111 & 112); General Biology I and II (BIO 111 & 112); Organic Chemistry I and II (CHE 231 & 232); Calculus I (MAT 111).

Course Objectives:

Students of this course will be assisted to

(1) Explain basic concepts of job input, output, scientific computing, and job submission.

(2) Explain techniques used in computational chemistry and molecular modeling.

(3) Use semi-empirical, *ab initio* and density functional theory (DFT) approaches to the representative problems of chemical interest, such as atomic and molecular structure and the properties of molecules.

(4) Determine how the energy of the system varies as the positions of the atoms and molecules change.

(5) Explain the conformational analysis and its importance to the physical, chemical and biological properties of a molecule.

(6) Learn about empirical force field models (also known as molecular mechanics) and its application to perform calculations on systems containing significant number of atoms.

(7) Compute the potential energy surface for representative molecules.

(8) Build peptides and explain some basic principles of protein structures, sequence analysis and protein folding.

(9) Lean the use molecular modeling and cheminformatics approaches to drug design in pharmaceutical industry.

(10) Use data science techniques to illustrate data relevant to social change issues and interpret the results.

(11) Appreciate research through reading journal articles and selected book chapters.

Learning Outcomes:

Upon successful completion of this course, students will be able to

(1) Employ the concepts and techniques used in computational chemistry and molecular modeling.

(2) Apply semi-empirical, *ab initio* and density functional theory (DFT) methods for calculations of molecular structures, energetics and electronic properties of chemical and biological systems.

(3) Perform calculations for the intermolecular interactions, conformational analyses of acyclic molecules and build polypeptides.

(4) Report and analyze results of their calculations

(5) Apply self-confidently for higher education on computational-based research in science or engineering fields, data science and be ready for the advanced level courses related to Computational Chemistry and Molecular Modeling.

Required Text:

Molecular Modelling: Principles and Applications, Andrew R. Leach, **Second Edition**, Pearson, England. (ISBN: 0-582-38210-6)

Reading assignments are as noted in the course schedule.

Teaching/Learning Methods/Classroom Format: *(lectures, videos, outside speakers, etc.)*

The class will be taught **primarily by lecture and demonstration**. A three hour / week lab associated with this lecture is offered. A significant amount of class participation is expected and required. A topic will be introduced and/or reviewed assuming that the students of this class have read the appropriate sections of the text before coming to the class. The material will then be developed further in the class by the instructor and/or students.

Problem Based Learning (PBL): Students will be grouped into teams. Each team will have 2 or 3 students to solve problems both inside and outside the classrooms and/or to complete the project. The team-based problem-solving approach is one of the High-impact Educational practices (Collaborative Learning Assignments and Projects). Individual assignments of problems will also be given.

Just-in-Time Teaching (JiTT) is a pedagogical strategy that uses feedback between classroom activities and work that students do at home, in preparation for the classroom meeting. It is timely pre-instruction assignments, usually called warm-ups that inform the upcoming lesson by encouraging the students to examine their prior knowledge and seek information about the upcoming topic before coming to class. JiTT improves student learning and increases in-class teaching efficiency and effectiveness, specifically, improves students' preparation for class, enhances student motivation for learning, promotes ongoing formative assessment of student learning (by both instructors and students), and informs in-class activities that target student learning gaps. Instructor will post question online (**CANVAS**) for students to respond online a few hours before class. JiTT questions are generally open-ended and require students to do something - read a textbook chapter or article, analyze a video, complete a simulation, or analyze data - related to material that will be addressed during the next class period.

Further details:
(1) **Videos of lectures** will be posted to students through canvas and/or using YouTube.

(2) Students will be strongly encouraged to share the muddiest point after each chapter through the canvas. The Muddiest Point is one of the simplest **Classroom Assessment Techniques** (CATs) to help assess where students are having difficulties. The technique consists of asking students to jot down a quick response to one question: “What was the muddiest point in [the lecture or discussion or homework assignment, etc.]?” The term “muddiest” means “most unclear” or “most confusing.”

As a High-impact Educational Practice, “**Undergraduate Research**" will be introduced to students. Instructor will reveal the importance of computational chemistry and molecular modeling research, publications, and the importance of starting research at early stage as well as potential opportunities to perform research at various institutions. Student teams will be engaged in collecting at least two research articles related to computational chemistry and molecular modeling. They will be asked to read, understand, discuss and prepare a mini report and final presentation for the project. In addition, students will be introduced to data science. Each team will use data science techniques to complete the assigned project relevant to social change issues and interpret the results. Computational chemistry part will be graded 50% and the **data science application** relevant to social change and interpretation of results will be graded 50%. **Each team will submit the report and presentation. Also, the team will deposit their oral presentation (25 minutes of presentation) in canvas**.

Assignments:

Standard rules of academic honesty apply. Penalties may be assessed if they are not followed. Individual or group assignments will be given. Homework is generally assigned for each chapter. In the starting of the semester, students will be grouped as teams. Each team should complete the assignment and submit through canvas before the due date. Late submissions will not be graded or be reduced the grade points. Successful completion of the assignments is imperative since enormous practice of applying the concepts of computational chemistry and molecular modeling to real problems is what finally makes the concepts intuitive. In this course, students will be given 2-4 assignments. Assignments should be submitted before the due date to be graded. Late submissions **will not be graded**. Since we plan to implement **Flipped Classroom** for this course, students will sometimes work inside the class to solve the homework assignments and students will get help from the instructor and/or TA.

Course Grading:

Three (3) written examinations (each 75-90 minutes exam for 50 points) will be given during the semester excluding final. Two best scores out of three exams will be considered for final grading. Thus, there **will not be any reexam or separate exam** for any student who had any kind of personal tragedy, ***from very serious to forgetting to set your alarm clock***. These exams are given after completing certain chapters and sections. Final exam will be comprehensive, and it will be conducted as per university schedule and will be given for **100 points**. The completion and submission of reports on or before the due dates for the **Computational Chemistry and Molecular Modeling Labs** will be evaluated for 180 points. Quiz will be given through **canvas** and inside the class, and students can expect 5-7 quizzes. Total points for all the quizzes will be converted to 100 points that will also be included for final grading. Quizzes will have timeframe and all students must finish the quizzes within the time otherwise **no second chance** to complete the quizzes. Students who have attended first lecture or followed the instructions and completed all activities assigned to students before the due dates will earn 20 points and others will **not** receive any points. Total points for all assignments will be 100 (total of 3-4 assignments). Students will be given final project (team project) based on the research article from the journals and the data science application relevant to social change. The submission of report (as team) and final presentation (team) will be graded to 100 points. The **rubrics** (assessment tool) for the mini report and the presentation will be given later. Student's individual score out of **700 total points** will determine each student's final grade. The grading scheme that is typically used is as follows.

Description	Points	Percentage
Written Examination (The best of two exams)	100	14.3 %
Final Examination	100	14.3 %
Computational Chemistry & Molecular Modeling Lab	180	25.7 %
Cumulative Quiz Grade (total points from all quizzes)	100	14.3 %
Assignments	100	14.3 %
Attendance	20	2.8 %
Final project (Report & presentation)	100	14.3 %
Total	**700**	**100.0 %**

Score Percentage	Grade
90 – 100 %	A
80 – 89 %	B
70 – 79 %	C
60 – 69 %	D
0 – 59 %	F

Course Policies and Expectations:

The success of the course in reaching its stated goals is evaluated by the ability of the students to use the material presented in the course to solve real problems on exams and homework assignments. This is not a perfect method of evaluation because many factors other than a student's grasp of the material play a large role in his/her performance, particularly on an exam. However, these evaluation techniques are relatively objective and do give an approximate indication of the success of the students in learning and applying the material.

Attendance in class (synchronous) is encouraged for the online course. **No makeup** will be given for quizzes at any circumstance. Students are encouraged to ask questions in the class. **Do not hesitate to ask** about subject materials that are not clear. For more help or questions, contact me in person during my office hours or by e-mail. If you can't come during my office hours, please get my appointment for another time.

Exam Policy: Standard rules of academic honesty apply to exams. Penalties will be assessed if these are not followed. **Cheating** in the exam by copying from other students or from internet using cell phone or smartphone and/or iPad will be subject to the juristic action under the student's handbook. Consequently, the student will forfeit the grade received on the test and receive an "**F**" in its place and the final grade may also be "**F**" for that student. Students **must switch off smart phone or iPhone or iPad and keep inside bag** during exams. These devices should not be used as substitute for calculator. Students must bring calculator to the exams. Students are expected to arrive on time for exams. The instructor is under no obligation to provide extra time for a late-arriving student to complete the exam. Unless otherwise stated in advance, all exams, including the final exam, will be closed-book and closed-note exams. When needed, the instructor will provide tables of physical constants and character tables and scratch papers. Exams may be scheduled outside of the regular class time.

Problem Solving and Success in this Course: Based on the instructor's experience, one of the most effective ways of mastering the subject matter of this course is by solving problems. Students are strongly advised to work individually/team on the assigned problems and as many other relevant problems as possible. Students are reminded that working on problems is a much more effective way of learning than staring at the instructor's or someone else's solutions. If students encounter difficulties with problems, they are encouraged to consult the instructor or other students for help. However, each student's final written solutions of assigned problems must be written in his or her own words and must not be essentially a copy of another student's solution.

Class Regulations & Preparation:

(a) Students **MUST PREPARE** the corresponding chapter sections before the class. Students **are expected to read the textbook** regularly (recommend 4-5 hours reading per week) and carefully listen the lecture through online
(b) Class attendance is encouraged. Students are expected to be on time to the online class meeting and lab demo if applicable.
(c) Students should not cheat for exams, assignments, and quizzes. They should follow the expectations of the course.
(d) Recorded lectures will be posted on canvas.
(e) Instructor will capture pictures and videos during the class, assignment and exams as per university guidelines and policy. The pictures and videos are only for academic purposes that includes academic honesty. If you accept to be in this class, you provide us the permission to record and release to the public/CAU community.

Special Accommodations:

Clark Atlanta University is committed to providing students with a documented disability an equal opportunity to pursue a college education. Efforts will be made to meet requests for reasonable accommodations for those eligible under the Americans with Disabilities Act (ADA) of 2008, the Rehabilitation Act of 1973 and Section 504. Students with disabilities are encouraged to contact the Office of Counseling and Disability Services at (404-880-8044) located on the 3rd floor of Trevor Arnett Hall to discuss accommodations. Once reasonable accommodations are determined, it is the student's responsibility to present the Letter of Accommodation from The Office of Counseling and Disability Services to their professors.

Supplemental Readings/Additional Bibliography:
Students will be asked to find articles relevant to computational chemistry and molecular modeling for the **project** from the journals.

http://pubs.acs.org/ (American Chemistry Society Journals)
Journal of the American Chemical Society, *Journal of Physical Chemistry A*, *Journal of Physical Chemistry B*, *Journal of Physical Chemistry C*, *Journal of Chemical Theory and Computation*.

Course Outline and Schedule: *(dates, weeks, topics)*

Date	Day	Week	Topics	Section #
	TH	1	Introduction to Computational Chemistry Course	
	T	2	Useful Concepts in Molecular Modelling	1.1-1.6
	TH		Useful Concepts in Molecular Modelling – Mathematical Concepts	1.7-1.10
	T	3	An Introduction to Computational Quantum Mechanics	2.1-2.3
	TH		An Introduction to Computational Quantum Mechanics	2.4-2.5
	T	4	An Introduction to Computational Quantum Mechanics	2.6-2.7
	TH		An Introduction to Computational Quantum Mechanics	2.8-2.10
	T	5	Advanced ab initio Methods, Density Functional Theory and Solid-state QM	3.1-3.2
	TH		Advanced ab initio Methods, Density Functional Theory and Solid-state QM	3.3-3.4
	T	6	**Exam 1**	
	TH		Advanced ab initio Methods, Density Functional Theory and Solid-state QM	3.4-3.5
	T	7	Advanced ab initio Methods, Density Functional Theory and Solid-state QM	3.6
	TH		Advanced ab initio Methods, Density Functional Theory and Solid-state QM (**Density Functional Theory**)	3.7
	T	8	Advanced ab initio Methods, Density Functional Theory and Solid-state QM (**Density Functional Theory**)	3.8
	TH		Advanced ab initio Methods, Density Functional Theory and Solid-state QM (3.9 *The Future Role of Quantum Mechanics:* ***Theory and Experiment Working Together***)	3.9
	T	9	Empirical Force Field Models: Molecular Mechanics	4.1-4.3
	TH		Empirical Force Field Models: Molecular Mechanics	4.4-4.7
	T	10	Empirical Force Field Models: Molecular Mechanics	4.8-4.10
	TH		Energy Minimisation and Related Methods for Exploring the Energy Surface	5.1-5.2
	T	11	Energy Minimisation and Related Methods for Exploring the Energy Surface	5.3-5.5
	TH		Energy Minimisation and Related Methods for Exploring the Energy Surface	5.6-5.9
	T	12	**Model Computational Chemistry Project – Presentation by Expert / Professor**	
	TH		Conformation Analysis (**Exam 2 – Take Home**)	9.1-9.4
	T	13	Conformation Analysis	9.5-9.7
	TH		Conformation Analysis	9.8, 9.9, 9.11
	T	14	Protein Structure Prediction, Sequence Analysis and Protein Folding	10.1-10.3
	T		Protein Structure Prediction, Sequence Analysis and Protein Folding	10.4, 10.5
	TH	15	Protein Structure Prediction, Sequence Analysis and Protein Folding	10.6-10.9
	T		**Final Project Presentation**	
	TH	16	**Reading Period**	
	T		**Final Examination (Comprehensive)**	

Computational Chemistry and Molecular Modeling Lab

The lab associated with the course "Introduction to computational chemistry and molecular modeling" concentrates on computational modeling in chemistry and biology applications. The main purpose of this lab is to apply the techniques taught in the course and to gain in-depth knowledge through hands on training. Students will learn from this lab how the techniques can be used to study physical, chemical, and biological phenomena. Computational chemistry and molecular modeling lab will focus on constructing small chemical and large biological molecular model systems, and to study the intra- and inter-molecular interactions. Students will employ mainly quantum mechanical techniques (*ab initio* and DFT methods) in this course. Students will be taught how to analyze the results. They will gain some practical experience of the applications of computers in chemistry and biology. Students will use supercomputers for performing calculations relevant to the labs.

Learning Outcomes of the Laboratory Course:

Upon successful completion of this lab, students will be able to

(1) Apply *ab initio*, density functional theory and semi-empirical methods for calculations of molecular structures, physical, chemical, and biological properties.
(2) Perform calculations of geometry optimizations and vibrational frequencies for simple molecules.
(3) Perform calculations involving small peptides and protein structures and examine the amino sequences.
(4) Report and analyze results of their calculations
(5) Apply self-confidently for higher education on computational-based research in science or engineering fields and be ready for the advanced level courses related to Computational Chemistry and/or the broad area of Computational (Data) Science.

Grading of Lab Activities and Lab Reports:

This laboratory course requires writing-intensive or type the formal report with high quality pictures / figures in Microsoft Word. Graphs should be generated using Microsoft Excel when required. **If the student does not listen to professor or teaching assistant (TA) in the lab, he/she will be asked to leave and his/her grade for that specific lab will be zero**. The preparation of a formal lab report is a very important aspect of this lab. A formal lab report is due one week after the completion of each lab experiment. The report should contain **abstract**, **introduction**, **computational details**, **results and discussion**, and **conclusion**. Outside references (journal article or book / chapter in book) are expected to be included in the lab report. Template for laboratory report will be provided. It is required to type the reports and submit through **canvas**. Each formal report is graded for 30 points. Penalty of three (3) points/week will be assessed for reports turned in late. Five (5) labs with formal lab reports will be graded to **150 points** [5 x 30 points].

Date	Topics	Grade points
Aug. 30 - Sep. 12	Mathematical Concepts, Writing Z-matrix, Supercomputer access and job submission	30 pts
Sep. 13-26	Run calculations for small molecules: ethene, ethane, butane and benzene	30 pts
Sep. 27 - Oct. 10	Calculations using *ab initio* Methods, Density Functional Theory (DFT)	30 pts
Oct. 11-24	Hunter and Sanders rules – Aromatic-Aromatic Interactions	30 pts
Oct. 25 – Nov. 7	Hydrogen bonds, thermodynamics – Base pairs	30 pts
Nov. 8-14	Vibrational frequencies (water, glycine, alanine & polypeptides (peptide of 5 alanine residues and another peptide of 5 glycine residue)	30 pts

About Your Professor:

My name is Dr. Dinadayalane Tandabany. You may call me Dr. Dina or Dr. Tandabany according to your convenience. I am an **Associate Professor** in the Department of Chemistry. I am the Principal Investigator (PI) of two projects funded by the National Science Foundation (NSF). In addition, I serve or served as co-PI of the collaborative grants funded by Department of Energy and NSF. I lead the research lab and group of "**Computational Chemistry and Nanoscience**". I teach / taught graduate level courses of Thermodynamics, Quantum Mechanics, Molecular Spectroscopy, Physical Organic Chemistry and undergraduate level courses of Introduction to Computational Chemistry and Molecular Modeling & Lab, Physical Chemistry & Lab, General Chemistry I and II. Prior to joining Clark Atlanta University in January 2014, I was a Research Professor at Jackson State University, Jackson, MS where I taught General Chemistry, Quantum Chemistry, Atomic and Molecular Spectroscopy. I earned my **Ph.D. degree** in chemistry from Pondicherry University, India in 2005. In my Master's (M.S.) in Chemical Sciences, I studied Physical Chemistry, Inorganic Chemistry, Organic Chemistry, Spectroscopy, Solid State Chemistry, Quantum Chemistry, Group Theory, etc. My research areas are computational chemistry and computational materials science. I received number of awards including **"2019 BEYA STEM Innovator Award"** and was recognized for my achievements and services. In my research career, I have co-authored nearly **sixty (60) peer-reviewed publications** in highly reputed journals in the areas of nanomaterials/nanoscience, theoretical/computational chemistry, physical chemistry, organic chemistry, and physical organic chemistry. In addition, I am a co-author of **several book chapters** that were published by Royal Society of Chemistry, Elsevier, Springer, etc. I am always interested to perform high-quality research involving both graduate and undergraduate students in **Computational Chemistry** focusing on rapidly developing research areas of nanomaterials, weak interactions, and reaction mechanisms. I serve in the editorial board as well as reviewer board of the journals. I am a **reviewer** for approximately **forty (40)** internationally well-recognized journals. My publications received more than **1900 citations** with an ***h*-index of 25**. To know further about me and my **research publications** and citations, please follow the links given below.

http://scholar.google.com/citations?user=Y9MAIjUAAAAJ&hl=en

http://www.linkedin.com/pub/tandabany-c-dinadayalane/22/749/247

http://www.researchgate.net/profile/Tandabany_Dinadayalane2

ORCID ID: orcid.org/0000-0002-5007-6615

Any Additional Items Needed:

Laptop / personal computer to access the supercomputer and the scientific calculator.