Overview: This is a team and project oriented class, which will require significant work outside of class for you and your team. This class structure might not be for you. Think carefully about whether you will be able to tackle a course structured in this non-traditional way. Because of the course structure auditing is not permitted.

Requirements: Basic quantum mechanics and statistical mechanics. Access to a laptop or computer is required. Basic understanding of UNIX is also expected. For a quick UNIX tutorial see http://www.ee.surrey.ac.uk/Teaching/Unix/.

Computer accounts: Obtain an HPC account at https://icer.msu.edu/users/getting-started. This account will allow you to run Gaussian and AMBER, as well as other packages, during the course of the semester. You will need to have access to the HPC center through a laptop or desktop machine connected to the internet via WiFi or a landline. It is recommended that you obtain a copy of Molden for molecular structure building and graphics at http://www.cmbi.ru.nl/molden/molden.html. For proteins PyMol or VMD are suitable programs to use for visualization purposes.

Required Textbook:

Suggested Textbooks (not exhaustive):
Computational Chemistry
“Introduction to Computational Chemistry” F. Jensen.
“Molecular Modelling: Principles and Applications” A. Leach
“Molecular Modelling for Beginners” A. Hinchliffe
Quantum Mechanics
“Modern Quantum Chemistry: Introduction to Advanced Electronic Structure Theory” A. Szabo and N. S. Ostlund.
“Ab Initio Molecular Orbital Theory” W. J. Hehre; L. Radom; P. Schleyer and J. A. Pople.
“Approximate Molecular orbital Theory” J. A. Pople and D. Beveridge
Simulations
“Computer Simulation of Liquids” M.P. Allen and D. J. Tildesley
“Molecular Modeling and Simulation” T. Schlick
“The Art of Molecular Dynamics Simulation” D. Rapaport
“Dynamics of Proteins and Nucleic Acids” J. A. McCammon and S. C. Harvey

Course goals: To provide a basic theoretical understanding of computational chemistry and biology methodologies. This class is a project based class and it is expected that students will familiarize themselves with basic theoretical concepts via reading the course textbook. You will be tested on the outside reading via a take home exam for the course. The project portion of the course will involve the identification of a computational problem and its execution utilizing appropriate software. Focus of the project portion of the class will be on the correct and effective use of two basic computational chemistry programs: Gaussian (for quantum mechanical calculations) and AMBER (for classical molecular simulations). Other packages may be utilized depending on the goals of your project.

Project Plan:
1) Obtain appropriate HPC accounts
2) Set up project teams
3) Select a computational project
4) Execute the project
5) Analyze the results
6) Present and write-up the project

Grading: There will be one take home exam. The exam will be circulated early in the semester and will be due one week before the end of the class. The results from the project will be graded via your team presentation and by the write-up your team provides. Grading will also include a class participation component. Office hours will be by appointment.

Additional Class Policies

Diversity and Inclusion Policy
Inclusion and diversity are core values of MSU and the College of Natural Science. As Spartans, we are dedicated to respecting people of all backgrounds, beliefs, identity status, and political beliefs. The college is committed to creating a safe, supportive, and welcoming environment where all students, faculty, and staff can pursue academic and professional success. All members of the MSU community deserve each other’s respect, support, recognition, and protection. It is essential that we all work together to foster an inclusive community where Spartans of all backgrounds can study, work, and thrive.

Americans with Disabilities Act Accommodations
Michigan State University is committed to providing equal opportunity for participation in all programs, services, and activities. Requests for accommodations by persons with
disabilities may be made by contacting the Resource Center for Persons with Disabilities by phone at 517-884-RCPD or through the web at rcpd.msu.edu. Once your eligibility for an accommodation has been determined, you will be issued a verified individual services accommodation (“VISA”) form. Please present this form at the start of the semester and/or at least two weeks prior to the accommodation date. Requests received after this date will be honored whenever possible.

Policy Regarding Academic Dishonesty
Academic dishonesty of any kind will not be tolerated in this course. Please see the following website for information regarding Michigan State University’s policy regarding academic dishonesty:

https://www.msu.edu/~ombud/academic-integrity/index.html

Name and Pronoun Preference
All people have the right to be addressed and referred to in accordance with their personal identity. Please advise me of preferences early in the semester so that I may make appropriate changes to my records. Information on MSU’s preferred name policy: http://lbgrtc.msu.edu/trans-msu/msu-preferred-name-policy/.

Policy on Religious Observance
It is an MSU policy to permit students to observe holidays set aside by their chosen religious faith.

https://reg.msu.edu/ROInfo/Notices/ReligiousPolicy.aspx

If you absent yourself from class on your religious holiday, please make arrangements with me in advance.

Grief Absence Policy
Please visit MSU Grief Absence Policy:

https://reg.msu.edu/ROInfo/Notices/GriefAbsence.aspx

Please speak directly to me to let me know what has happened.

MSU - Mandatory Reporting Policy
As a professor, one of my responsibilities is to help create a safe learning environment for my students and for the campus as a whole. As a member of the university community, I have the responsibility to report any instances of sexual harassment, sexual violence and/or other forms of prohibited discrimination that I hear about.

If you would rather share information about sexual harassment, sexual violence or discrimination to a confidential employee who does not have this reporting responsibility, you can find a list of those individuals here https://caps.msu.edu/