The University of Western Ontario  
Department of Chemistry  

Chemistry 3300B  
COMPUTER METHODS IN CHEMISTRY  
Winter 2024 (tentative)  

Course Information  

Instructor: Viktor N. Staroverov  
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Office: ChB 063  

Lectures: Monday, Wednesday, Friday, 10:30 am - 11:30 am, ChB 9  
Tutorials: Approximately every other week on Tuesdays, 1:30 pm - 3:30 pm, SSC 1000  
Office hours: By appointment (administrative matters)  
Course web site: https://owl.uwo.ca/portal  

Prerequisites: Chemistry 1301A, Chemistry 1302B, and any 1.0 courses at the 1000 level or higher from Calculus, Applied Mathematics or Mathematics, with no mark less than 60% in any of the above. Integrated Science 1001X with a minimum mark of 60% may be used as a substitute for (Chemistry 1302A/B and Calculus 1301A/B).  

Description: An introduction to computer methods and tools used in all branches of chemistry. Topics include molecular structure visualization, calculation of molecular structure and properties, analysis of reaction mechanisms using potential energy surfaces, simulation of molecular spectra, numerical methods, data processing, and symbolic computation software.  

Course Topics  

Expected Learning Outcomes

- Recognize the utility of computer tools in chemistry research
- Understand the basic theoretical principles of molecular structure calculations
- Visualize, build, and manipulate molecular structures on a computer
- Understand the origin and meaning of molecular orbitals
- Know how to use the Gaussian program to predict the most stable structures of molecules, calculate reaction enthalpies and Gibbs energies, simulate vibrational spectra, correlate electronic structure with chemical properties
- Be able to perform basic operations of calculus and linear algebra using Maple
- Be able to perform least-squares fitting and regression analysis of data using Excel
- Be aware of the capabilities and limitations of computational chemistry techniques

Course materials: There is no required text. All course materials (lecture notes, manuals, etc.) will be distributed via the course website.


Evaluation: The course grade will be determined as a weighted average of the following components:

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<thead>
<tr>
<th>Component</th>
<th>Weight</th>
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<tbody>
<tr>
<td>Tutorials</td>
<td>30%</td>
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<tr>
<td>Assignments</td>
<td>16%</td>
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<tr>
<td>Midterm test</td>
<td>14%</td>
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<td>Final exam</td>
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Tutorials 30% (5% each)
Assignments 16% (4% each)
Midterm test 14%
Final exam 40%