**Instructor:** Dr. Kostas Vogiatzis  
**Office:** Bu 319; Office Hours (open door or by appointment)  
**Phone:** N/A

**Textbooks:**  
A. "Spectra of Atoms and Molecules; Second Edition"  
   Peter F. Bernath (Oxford University Press, New York, NY 2005).  
B. “Modern Quantum Chemistry”  
C. “Molecular Electronic Structure Theory”  

**Grading:**  
Midterm Exam: 25%  
Final Exam: 25%  
Problem Sets: 25%  
Computational Exercises: 25%

**Class Schedule:** Every Tuesday and Thursday, 11:10-12:25, Buehler 472

**Topics:**  
1. Modern electronic structure theory  
2. The electromagnetic spectrum, characteristics of radiation  
3. Symmetry and group theory  
4. Introduction to rovibrational spectroscopy  
5. Electronic spectroscopy for atoms and molecules  
6. Computational chemistry and spectroscopy

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<td>Modern Electronic Structure Theory (Chapters from books B and C)</td>
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<td>Introduction - Foundations of Molecular Orbital Theory</td>
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<td>Exact and Approximate Wave Functions</td>
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<td>Atomic Basis Functions and Basis Sets</td>
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<td>Multiconfigurational Quantum Chemistry</td>
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<td>II.</td>
<td>Electromagnetic Interactions (Book A, Chapter 1)</td>
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<td>Charge Distributions and their interaction with radiation fields</td>
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<td>1</td>
<td>Weak Field Electromagnetic Radiation and Optical Transitions</td>
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III. Symmetry and Group Theory (Book A, Chapters 2-4)

1. Symmetry Operators and Point Groups

2. Matrix Representation of Operators and Groups

2. Quantum Mechanics and Group Theory

IV. Rotational Spectroscopy (Book A, Chapter 6)

1. Structure and Rotation of Rigid Bodies

1. Pure Rotational Spectra of Diatomics and linear Polyatomics

V. Vibrational Spectroscopy (Book A, Chapters 7-8)

1. Vibrational Wavefunctions and Energy Expressions

1. Vibrational-Rotational Spectra in Diatomics

2. Polyatomic Normal Modes and Vibrational Transitions

1. Raman Spectroscopy

Calculation of rovibrational spectra of diatomic molecules

VI. Electronic Spectroscopy of Diatomic Molecules (Book A, Chapter 9)

1. Molecular Orbitals, Configurations and States - Vibrational Fine Structure in an Electronic Transition

1. Rotational Fine Structure in a Vibrational Transition

VII. Electronic Spectra of Polyatomic Molecules (Book A, Chapter 10)

1. Molecular Orbitals, Configurations and States

1. Electronic Structure and Spectra of Triatomic Molecules; Walsh’s Rules


1. Electronic Structure and Spectra of larger polyatomics

Calculation of adsorption spectra of polyatomic molecules

VIII. Computational Spectroscopy (Notes)

Total:
27 lectures
2 lectures dedicated to exercises and computational spectroscopy