

OSU Chemistry Graduate Course 7530, Fall 2018

## Structure and spectra of molecules

**Time and Location: Tue and Thurs, 2:20 – 3:40 pm**

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### Topics to be covered (tentative)

Theory: Newton's equation of motions

Example: Classical harmonic oscillator

Boltzmann probability distribution and Boltzmann entropy

Thermodynamics

Application: Atomic force microscopy in harmonic limit and beyond

Generalization: Harmonic oscillator in many-atom molecules

Normal mode analysis and elastic network models of macromolecules

Quasi-harmonic analysis/essential dynamics

Principal component analysis as a general tool for data mining

Machine learning and neural networks

Data clustering

Conformational entropy and entropy localization beyond the harmonic limit

Theory: Interaction of electromagnetic radiation with matter: electric effects

Application: rotational spectroscopy

Application: vibrational spectroscopy, IR spectroscopy, Raman spectroscopy

Application: electronic spectra

Theory: Interaction of electromagnetic radiation with matter:

magnetic effects

Application: magnetic resonance, Bloch equations in EPR and NMR

Theory: Linear response theory and Fourier spectroscopy

Time-domain analysis, Nyquist sampling

Multi-dimensional spectroscopy

Maximum entropy reconstruction, compressed sensing

Theory: Time-dependent quantum mechanics

the quantum-mechanical two-level system

Introduction to quantum-information theory: Bell's inequalities

Theory: Quantum-mechanical description of molecular ensembles, density matrix, pure vs. mixed states

Liouville-von-Neumann equation

Theory: Tensorial interactions and their irreducible representations

Theory: Quantum mechanics of open systems and dissipation

Time-correlation functions, spectral densities,

Wiener-Khinchin theorem

Markov processes, kinetic network models

Redfield theory, model-free approach  
Kubo theory and stochastic Liouville equation

Theory: Bayesian analysis of spectroscopic data, Markov Chain Monte Carlo  
Application: Probability distribution of model parameters from spectroscopic data

Special topics can be added in response to specific student interest.

## **MATLAB**

This course will involve computer programming applications using the MATLAB programming language. OSU has a site license for MATLAB, i.e. you can install it for free on your laptop or a computer in the lab of your advisor using the following instructions:

MATLAB® is available from MathWorks® for free to students and faculty at OSU through the office of the Chief Information Officer. MATLAB® is a high-level programming language and interactive environment used by millions of engineers and scientists worldwide. It can give you access to a vast range of powerful computational routines with a wide range of utility beyond this class and in your future career. To set-up MATLAB® on your own computer, go to <https://ocio.osu.edu/software>, choose your computer type, then choose "MATLAB" and follow the prompts. You will end up at the Office of the Chief Information Officer Self Service Site: <https://osuitsm.service-now.com/selfservice/>. Login with your OSU name.# credentials to obtain activation information. You basically get a sheet (\*.pdf) with activation information, then you go to the MathWorks' website to download and activate the software. Don't assume that you can set up MATLAB® an hour before homework is due. Set it up now while you have time and verify that you can access WebMO as well.

If you are new to Matlab or already know it, quickly establish your programming skills by going through some Matlab tutorials and exercises. As a graduate student in Chemistry you will invariably need to do computer programming for accomplishing your research and Matlab is a very powerful, intuitive, and easy-to-learn programming language. And it is fun too!

Tutorial (there are many others on the web that are quite good):

<http://www.math.toronto.edu/mpugh/primer.pdf>

I will also put my own tutorial online.

Also, when you have a question about Matlab, just google it. Since Matlab is very widely used worldwide, in all likelihood somebody already posted the answer to your question.