

### Lecture 3. Quantum Mechanics

- Download course materials  
<https://mulan.swmed.edu/lecture3.tar.gz>

*To unpack the tar.gz ball, run the following command:*

*`tar xvfz lecture3.tar.gz`*

*A new directory, lecture3 will be created*

- **Install the following software packages**
  1. Avogadro-1  
<https://sourceforge.net/projects/avogadro/files/avogadro/1.1.1/>
- Read the book chapter of “Molecular Modelling: Principles and Applications (2nd Edition)” entitled “An Introduction to Computational Quantum Mechanics” in lecture3/reading
- Go through the Gaussian 09 tutorials
  1. Run Gaussian 09 tutorial in lecture3/g09\_tutorial
  2. Use Avogadro to display the Gaussian outputs (orbitals, electron density, vibrational modes, etc.)