# CHEM 4010: Introductory Quantum Chemistry
## Learning Outcomes

1. Describe specific examples where classical mechanics (CM) fails completely to account for experimental observations, and describe how the predictions of quantum mechanics (QM) agree with those observations.

2. Describe in which ways quantum mechanics (QM) is more general and more reliable than classical mechanics (CM), and how QM becomes equivalent to CM in the limits of high temperature, high mass, and free motion (motion on a flat potential surface).

3. Apply the DeBroglie formula and related concepts to assess whether a system can be reliably described by CM or not. Identify chemical systems and processes where CM gives a completely adequate description, and chemical systems and processes where CM fails entirely to describe reality and where QM is needed.

4. Carry out simple calculations involving complex numbers, functions and operators.

5. Describe how the size and shape of a box, and the mass of a particle in it, influence the allowed energy states; calculate realistic energies for particle-in-a-box (PIB) systems.

6. Explain how the absorption of light can promote a transition from a QM energy state to another QM energy state, and describe in words, graphs, and equations the relation between an absorption spectrum and energy levels in an atom or molecule.

7. Model the energy states of various chemical systems with PIB concepts and equations. The chemical systems in question are: conjugated $\pi$ electron systems; bulk metals vs bulk semiconductors and insulators; atomic orbitals (AO), in particular the distinction between core, valence and Rydberg states; and the covalent bond in $H_2^+$ and $H_2$.

8. Predict trends in the UV-vis absorption frequency of atoms (and some molecules) by using the QM-derived energy formula of the hydrogenoid atom; calculate realistic approximate absorption frequencies by applying that formula in various systems.

9. Give a qualitatively correct description of atomic orbitals (AO), and the molecular orbitals of small molecules, including the symmetry properties and nodal structure, the sign in different regions of space, and the asymptotic behavior.

10. Give a qualitatively correct description of the electron density in atoms and small molecules. Calculate the integrated electron density (electron count) in simple model systems.

11. Define ionization energy (IE) and electron affinity (EA). Give reasonable estimates of IE and EA in atoms and small molecules, and give reasonable predictions of trends.

12. Define electron removal energies, and give reasonable estimates by using the hydrogenoid AO energy formula and Slater's AO screening formula.

13. Predict trends in the infrared fundamental absorption frequency for diatomic molecules, and for small functional groups within polyatomic molecules, by using the QM-derived energy formula of an harmonic oscillator; calculate approximate fundamental absorption frequencies by applying that formula in various systems.

14. Predict trends in the microwave absorption frequency for various diatomic molecules by using the QM-derived energy formula of a rigid rotor; calculate approximate microwave absorption frequencies by applying that formula in various systems.

15. Define absolute electronegativity $\chi$ and hardness $\eta$, make realistic calculations or guesses of $\chi$ and $\eta$ in atoms and molecules, and make qualitative predictions about chemical reactivity and the ionic character of chemical bonds based on $\chi$ and $\eta$.

16. Explain what are a function, a functional, an operator, a vector, and a matrix.

17. Describe the analogy between function and vector, matrix and operator.

18. Explain the concepts of a basis of vectors, a basis of functions, orthogonality and normalization of functions. Describe how the use of a basis of functions to approximate wavefunctions transforms the Schrödinger equation into a matrix eigenvalue equation.

19. Describe the Huckel hamiltonian matrix model, and give realistic numerical values, in eV, for the matrix elements of the Huckel hamiltonian in simple $\pi$-conjugated molecules.

20. Reading from the output of a Huckel calculation — in particular the matrices E, C, and $CNC^\dagger$ — give a sensible description of the electronic structure in the molecule. What are the bond orders? What are the atomic charges? What do the frontier orbitals look like?

21. Explain the Born-Oppenheimer approximation and what a potential energy surface is. Without too many details, give a step-by-step description of how a software like "Gaussian" works to deliver the orbitals and orbital energies of density functional theory (DFT); give a simple description of the approximations and methods involved.

22. Reading from the output of a series of Gaussian DFT calculations, obtain theoretical predictions for: equilibrium bond lengths and bond angles; energies of reaction; ionization energies; electron affinities; the nature of frontier orbitals; the charge distribution within the molecule in its ground state.