

Screening Procedure Topics: Physical and Theoretical Section

The topics below are based on the following four required core courses (**Chem 544:** Introduction to Quantum Chemistry, **Chem 540:** Introduction to Statistical Mechanics, **Chem 535:** Introduction to Molecular Spectroscopy, and **Chem 538:** Mathematical Methods in Physical Chemistry). All students are expected to know these topics, regardless of their area of research. However, they may choose to present the application of a concept from their own area of research. Further in-depth knowledge of these and other specialized and advanced concepts as they pertain to their own specific research area will be discussed in the qualification exam, and not within this procedure. For each topic the students will be tested both on the conceptual foundation as well as the application.

1. Fermi's Golden Rule.

Application: Application of Fermi's golden rule to at least one problem (e.g. electron transfer, vibrational energy transfer, exciton transfer, spin transitions, spin diffusion, or any area that the student is working in).

2. Franck-Condon Principle.

Application: The consequences of Franck-Condon principle on the absorption spectrum of small molecules, or any system that the student is currently studying in his/her own research. Explanation of vibronic structure and Huang-Rys factors.

3. Born-Oppenheimer approximation and Potential Energy Surfaces.

Application: Describe the first few potential energy surface of a simple small molecule, or a molecule that the student is currently studying in his/her own research. Description of adiabatic vs. diabatic surfaces, curve crossing, Landau-Zener formula.

4. Einstein coefficients

Application: relationship between absorption, stimulated emission, and spontaneous emission (fluorescence); relationship between transition strength and radiative lifetime; population dynamics in optically pumped systems, including lasers.

5. Nuclear and electron magnetic resonance.

Application: Spin dynamics in magnetic resonance, including Bloch sphere picture for evolution of spin states, pulsed excitation, evolution of spins, decoherence, population decay, spin echo, free induction decay.

6. Time-dependent perturbation theory.

Applications: Interaction of light with two-level systems, Rabi oscillation, absorption and stimulated emission.

7. Model 1-D, 2-D, and 3-D systems. (particle in a box, harmonic and anharmonic oscillator, and hydrogen atom)

Applications: Quantum dots, 2-D materials, vibrational excitations in harmonic and anharmonic systems including selection rules,

8. Taylor series.

Application: Any application of Taylor series in quantum mechanics, optics, or electronic structure theory, including any from the student's own research (e.g. nonlinear optics)

9. Solutions of ordinary and partial differential equations.

Application: Any application of a first order or second order differential equation, including those pertaining to student's research (e.g. chemical kinetics, wave propagation, 1-D Schrodinger's equation).

10. Fourier transforms:

Application: Relation between linewidths and time, free-induction decay, beats between two frequencies, or any application in student's research (e.g. pulse shaping, interferometry, dispersion correction).

11. Eigenvalue/eigenfunction problems.

Applications: Diagonalization of a 2x2 Hamiltonian and its application in splitting of spectral lines (e.g. spin-spin coupling, exciton splitting, vibrational line-splitting). Band structures and extended solids arising from nearest neighbor coupling.

12. Boltzmann distribution.

Applications: Any application of the Boltzmann distribution in spectroscopy or in the student's research area (e.g. Raman thermometry, temperature dependent EPR and NMR, dynamic nuclear polarization, hot bands in vibrational spectroscopy, Poisson-Boltzmann description of screening, Debye-Huckel theory, Gouy-Chapman theory, Maxwell-Boltzmann distribution of molecular speeds).

13. Fermi-Dirac and Bose-Einstein distributions.

Applications: Excitations in metals and semiconductors, Fermi-level, charge transport in metals and semiconductors.

14. Ensembles and partition functions.

Applications: Multistate equilibrium systems. Calculation of properties averaged over a distribution with examples (e.g. heat capacity, electric or magnetic polarization, conductivity, low and high temperature limits of partition function of quantum harmonic oscillators)

15. Correlation functions:

Application: Linear and nonlinear spectroscopy, time-domain vs frequency-domain understanding of dynamics.