

Computer Simulations of Chemical Reactions in Solution and Biomolecules

MSc. and Ph.D. Course

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1. **Introduction to Molecular Modeling:** *Historical Developments, Literature*
2. **Quantum Mechanics I.:** *Key Concepts, Methods, and Machinery*
3. **Quantum Mechanics II.:** *Key Concepts, Methods, and Machinery*
4. **Molecular Mechanics:** *Key Concepts, Methods, and Machinery*
5. **Statistical Thermodynamics:** *Essential Concepts (Partition Functions, Boltzmann Population, Entropy, Enthalpy, Free Energy)*
6. **Solvation Methods:** *Polarized Continuum Methods (PCM), Conductor-Like Screening Model (COSMO, COSMO-RS), Explicit Solvation, PBSA/GBSA Methods*
7. **QM/MM Methods:** *Background, Theory, Applications, and Case Studies (Reaction Mechanisms of Enzymes)*
8. **Thermodynamic Cycles for Computation of a Free–Energy Change in Condensed Phase:** *Concepts, Applications (Reduction Potentials and Acidity Constants)*
9. **Free Energy Perturbation (Thermodynamic Integration) and PMF Methods:** *Concept, Theory, Applications*
10. **Transition State Theory:** *Eyring Equation (Theory, Applicability and Limitations, Kinetic Isotope Effects, Tunneling Correction), More Advanced Theories (Variational Transition State Theory)*
11. **Modelling Chemical Reactions in Solution:** *Theory and Applications*
12. **Physical Chemistry of Enzyme Catalysis I:** *Reaction Rate and Order, Michaelis-Menten Equation, Metals in Enzymology (Stability Constants, Selectivity, Magnetism, Spectroscopy, Redox and Spin-State Activity)*
13. **Physical Chemistry of Enzyme Catalysis II:** *Theoretical Calculations of Reaction Profiles, Electron Transfer Kinetics and Redox Reactions, Marcus Theory, Adiabatic versus Non-adiabatic reaction dynamics (Landau-Zener model and beyond)*
14. **Recent Advances in Molecular Modeling.** *Outlook and Summary.*

Talks by LR

Talks by MS