Essentials of Computational Chemistry: Theories and Models, 2nd Edition
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3. Simulations of Molecular Ensembles.

6. Ab Initio Implementations of Hartree-Fock Molecular Orbital.

Theory.

7. Including Electron Correlation in Molecular Orbital Theory.

8. Density Functional Theory.

11. Implicit Models for Condensed Phases.

12. Explicit Models for Condensed Phases.

References.

14. Excited Electronic States.

14.1 Determinantal/Configurational Representation of Excited States.

14.2 Singly Excited States.

14.2.1 SCF Applicability.

14.2.2 CI Singles.

14.2.3 Rydberg States.

14.3 General Excited State Methods.

14.3.1 Higher Roots in MCSCF and CI Calculations.

14.3.2 Propagator Methods and Time-dependent DFT.

14.4 Sum and Projection Methods.

14.5 Transition Probabilities.

14.6 Solvatochromism.

14.7 Case Study: Organic Light Emitting Diode Alq3.

Bibliography and Suggested Additional Reading.

References.

15. Adiabatic Reaction Dynamics.

15.1 Reaction Kinetics and Rate Constants.

15.1.1 Unimolecular Reactions.

15.1.2 Bimolecular Reactions.

15.2 Reaction Paths and Transition States.

15.3 Transition-state Theory.

15.3.1 Canonical Equation.

15.3.2 Variational Transition-state Theory.

15.3.3 Quantum Effects on the Rate Constant.

15.4 Condensed-phase Dynamics.