# CHAPTER OVERVIEW

## 8: Chemical Dynamics

**Learning Objectives**

In this Chapter, you should have learned about

- Conventional and variational transition state theory.
- Classical trajectory and reaction-path Hamiltonian simulations of chemical reactions.
- Unimolecular RRKM theory.
- Time correlation function and wave packet propagation approaches.
- Surface hopping and Landau-Zener theories of non-adiabatic processes.
- Spectroscopic, beam, and other experimental approaches to probing chemical reaction rates.

Chemical dynamics is a field in which scientists study the rates and mechanisms of chemical reactions. It also involves the study of how energy is transferred among molecules as they undergo collisions in gas-phase or condensed-phase environments. Therefore, the experimental and theoretical tools used to probe chemical dynamics must be capable of monitoring the chemical identity and energy content (i.e., electronic, vibrational, and rotational state populations) of the reacting species. Moreover, because the rates of chemical reactions and energy transfer are of utmost importance, these tools must be capable of doing so on time scales over which these processes, which are often very fast, take place. Let us begin by examining many of the most commonly employed theoretical models for simulating and understanding the processes of chemical dynamics.



### Contributors and Attributions

- Jack Simons (Henry Eyring Scientist and Professor of Chemistry, U. Utah) Telluride Schools on Theoretical Chemistry
- Integrated by Tomoyuki Hayashi (UC Davis)