CHAPTER OVERVIEW

3: Characteristics of Energy Surfaces

Learning Objectives

In this Chapter, you will learned about the following things:

1. Characteristics of Born-Oppenheimer energy surfaces, and how to find local minima, transition states, intrinsic reaction paths, and intersection seams on them.
2. The harmonic normal modes of vibration extracted from the mass weighted Hessian matrix, and how symmetry can be used to simplify the problem.

Born-Oppenheimer energy surfaces (or the empirical functions often used to represent them) possess important critical points that detail the properties of stable molecular structures, transition states, intersection seams, and reaction paths, all of which play central roles in the theoretical description of chemical reactions and molecular properties. In this Chapter, you will learn about these special points on the surfaces, how to find them, and what to do with them once you know them.

Contributors and Attributions

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