

<<理论化学导论>>

图书基本信息

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作者：Jack Simons

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## 内容概要

Let's begin by discussing what the discipline of theoretical chemistry is about. I think most young students of chemistry think that theory deals with using computers to model or simulate molecular behaviors. This is only partly true. Theory indeed contains under its broad umbrella the field of computational simulations, and it is such applications of theory that have gained much recent attention especially as powerful computers and user-friendly software packages have become widely available. However, this discipline also involves analytical theory, which deals with how the fundamental equations used to perform the simulations are derived from the Schrödinger equation or from classical mechanics, among other things. The discipline also has to do with obtaining the equations that relate laboratory data (e.g., spectra, heat capacities, reaction cross-sections) to molecular properties (e.g., geometries, bond energies, activation energies). This analytical side of the theory is also where the equations of statistical mechanics that relate macroscopic properties of matter to the microscopic properties of the constituent molecules are obtained.

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