

CHAPTER OVERVIEW

20: Response Theory

Many physical properties of a molecule can be calculated as expectation values of a corresponding quantum mechanical operator. The evaluation of other properties can be formulated in terms of the "response" (i.e., derivative) of the electronic energy with respect to the application of an external field perturbation.

[20.1: Calculations of Properties Other Than the Energy](#)

[20.2: Ab Initio, Semi-Empirical, and Empirical Force Field Methods](#)

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