

CHAPTER OVERVIEW

11: Computational Quantum Chemistry

Computational chemistry is the field of chemistry that uses mathematical approximations and computer programs to solve problems of chemical interest. Quantum chemistry is a subfield that addresses the equations and approximations derived from the postulates of quantum mechanics; specifically involving solving the Schrödinger equation for molecular systems. Quantum chemistry is typically separated into *ab initio*, which uses methods that do not include any empirical parameters or experimental data and semi-empirical which do.

[11.1: Overview of Quantum Calculations](#)

[11.2: Gaussian Basis Sets](#)

[11.3: Extended Basis Sets](#)

[11.4: Orbital Polarization Terms in Basis Sets](#)

[11.E: Computational Quantum Chemistry \(Exercises\)](#)

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