



# Electronic Structure Modeling: Connections Between Theory and Software

*Carl Trindle, Donald Shillady*

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Computational chemistry, including electronic structure modeling, is a fast and accurate tool for treating large chemically meaningful systems. Unique among current quantum chemistry texts, **Electronic Structure Modeling: Connections Between Theory and Software** enables nonspecialists to employ computational methods in their own investigations.

The text illustrates theoretical methods with numerical detail and model calculations. It clarifies what these modeling programs can do, their known pathologies, which ones are suited for specific kinds of projects, and how to reproduce them using the accompanying PC-LOBE bundled software. While elucidating gradient-based molecular structure optimization, the text reviews notable successes and unsolved problems or failures in electronic structure modeling. It also describes the theory and computation of circular dichroism and optical rotation, including magnetically induced optical phenomena.

Offering an accessible introduction to computational methods, **Electronic Structure Modeling** permits users to practice modeling with a full understanding of the algorithms that support their calculations.

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