



## Structure and Function

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The art of chemistry is to thoroughly understand the properties of molecular compounds and materials and to be able to prepare novel compounds with predicted and desirable properties. The basis for progress is to fully appreciate and fundamentally understand the intimate relation between structure and function. The thermodynamic properties (stability, selectivity, redox potential), reactivities (bond breaking and formation, catalysis, electron transfer) and electronic properties (spectroscopy, magnetism) depend on the structure of a compound. Nevertheless, the discovery of novel molecular compounds and materials with exciting properties is often and to a large extent based on serendipity. For compounds with novel and exciting properties, a thorough analysis of experimental data – state-of-the-art spectroscopy, magnetism, thermodynamic properties and/or detailed mechanistic information – combined with sophisticated electronic structure calculations is performed to interpret the results and fully understand the structure, properties and their interrelation. From these analyses, new models and theories may emerge, and this has led to the development of efficient models for the design and interpretation of new materials and important new experiments. The chapters in this book therefore describe various fundamental aspects of structures, dynamics and physics of molecules and materials. The approaches, data and models discussed include new theoretical developments, computational studies and experimental work from molecular chemistry to biology and materials science.

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