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Electronic Structure of Advanced Functional Materials

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Message from the Guest Editor

The Special Issue is divided into two parts: part I reviews the fundamental principles of the electronic structure of materials, while part II presents more specialized topics such as electronic structure analysis methods, band structure calculations of various functional materials, and the application of these materials in various fields.

In Part I, articles discuss theoretical approaches to understanding an electronic structure, such as density functional theory (DFT). Other topics covered include related concepts such as chemical bonding, molecular shape and symmetry, electron–phonon interactions, and other aspects of quantum chemistry.

Part II includes applications of electronic structure analysis methods to various materials such as perovskites, kaolinite, hectorite, barium titanate, and ferroelectric materials. In addition, the charge transport mechanism of organic–inorganic hybrid materials for optoelectronic devices is discussed. Moreover, future directions of research regarding advanced materials in photonics, spintronics, topological materials, and water splitting are highlighted.

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