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Application of First Principle Calculation in Metallic Materials

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Message from the Guest Editors

Compared with trial-and-error experiments, designing materials via the first-principles approach is highly desirable, as it saves significant time and money. The remarkable accuracy and sophistication of modern first-principles electronic structure methods are undoubtedly bringing us closer to this goal. While all materials properties are ultimately determined by chemistry and local atomic structure, many properties cannot be formulated as a direct prediction of the Schrödinger equation. Within the last few decades, a dramatic advancement has been achieved through the combination of first principles and statistical mechanics approaches that connect a crystal's thermodynamic and kinetic properties to its thermal excitations, such as configurational, vibrational, and electronic excitations, achieving phenomenological description at experimentally relevant length scales and timescales at minimal cost time.

This Special Issue will present interdisciplinary work aimed at understanding the essentials of chemistry and the atomic scale and designing materials using phenomenological description.

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Message from the Editorial Board

Metallic materials play a vital role in the economic life of modern societies; contributions are sought on fresh developments that enhance our understanding of the fundamental aspects related to the relationships between processing, properties and microstructure – disciplines in the metallurgical field ranging from processing, mechanical behavior, phase transitions and microstructural evolution, nanostructures, as well as unique metallic properties – inspire general and scholarly interest among the scientific community.

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