Special Issue

Advances in First-Principles Calculations on Metallic Materials

Message from the Guest Editor

Alloys, composed of several elements, form intermetallic compounds or solid solutions. Solid solutions are chemically disordered crystalline materials. The random distribution of elements results in the large degree of uncertainty and further induces a great fundamental challenge to conventional ab initio calculations. In short, one can't use a simple structural model to simulate alloys. The supercell and effective medium methods were proposed to simulate successfully the chemical and magnetic disorder in alloys. Similar to the importance of XRD in experiments, ab initio calculations in theory have been become a powerful tool to investigate the intrinsic properties of metals and alloys. The Special Issue includes, but is not limited to the following areas:

- Ab initio based methods on metals and alloys
- Intrinsic properties, such as electronic structure, elastic constants, elastic moduli, stacked fault energy, surface energy, interface energy, thermodynamic properties, phase transformation, etc.

Guest Editor

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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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