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Ab Initio Study of Metallic Materials

Guest Editor:

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Deadline for manuscript submissions:
closed (30 June 2021)

Message from the Guest Editor

Dear Colleague,

Quantum-mechanical (also called ab initio or first-principles) calculations have recently become a well-established tool for all materials scientists who are interested in phenomena occurring at the nanometer and sub-nanometer scale. Quantum-mechanical approaches have become the method of choice not only for studying existing materials but also for designing new ones. Importantly, whenever experimental data are missing or impossible to obtain, first-principles calculations represent the only source of information.

This Special Issue covers all applications of ab initio methods to problems related to metallic materials, including their electronic, magnetic, elastic as well as other properties, thermodynamic and mechanical stability, kinetics, strength, plasticity mechanisms, point-/extended defects (vacancies, dislocations, grain boundaries, etc.), transitions, as well as phenomena occurring in their lower-dimensional states or multi-phase composites (interfaces).

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Message from the Editor-in-Chief

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