Special Issue

Ab Initio Study of Metallic Materials

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).

Guest Editor

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Deadline for manuscript submissions

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Message from the Editor-in-Chief

Materials (ISSN 1996-1944) was launched in 2008. The journal covers twenty-five comprehensive topics: biomaterials, energy materials, advanced composites, advanced materials characterization, porous materials, manufacturing processes and systems, advanced nanomaterials and nanotechnology, smart materials, thin films and interfaces, catalytic materials, carbon materials, materials chemistry, materials physics, optics and photonics, corrosion, construction and building materials, materials simulation and design, electronic materials, advanced and functional ceramics and glasses, metals and alloys, soft matter, polymeric materials, quantum materials, mechanics of materials, green materials, general. *Materials* provides a unique opportunity to contribute high quality articles and to take advantage of its large readership.

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