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First-Principles Approaches to Metals, Alloys, and Metallic Compounds

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Current fundamental electronic-structure theory allows for the accurate prediction and characterization of elemental metals adopting any allotropic structure, intermetallic compounds, and other metal-rich phases. From an engineering perspective, there is a need for structural materials that are suitable for mechanical and civil engineering as well as energy production and conversion. While different microstructural features influence the macroscopic behaviour, quantum-mechanical simulation may enormously accelerate and guide the entire development process since atomistic modelling allows for the generation of structural models and the calculation of enthalpies and other free energies as a function of pressure and temperature. Among other things, this volume covers high-manganese steels, some of which have come to light within Collaborative Research Centre 761 (“Steel ab initio”). In particular, it deals with short-range ordering from experiment and theory, also highlighting carbide-like precipitates, and it bridges the gap between atomistic and continuum levels, in particular for hydrogen embrittlement. Molecular dynamics simulates crack propagation, and first-principles theory helps in growing better intermetallic thin films and predicts structural and elastic properties. Eventually, multiscale modelling of hydrogen transport is provided, and the chemical reasons for H-trapping κ -carbides are highlighted. First-principles theory has acquired a powerful role in the fundamental and applied research of metals, alloys, and metallic compounds.

