Special Issue

First Principles Simulations of Minerals

Message from the Guest Editor

The purpose of this Special Issue is to highlight recent advances and examine future directions in the study of minerals relevant to geophysics and planetary science using first principles techniques. Examples include high pressure transitions, melting curves, equations of state, phase diagrams, elastic, and transport properties. As these properties remain largely unconstrained at high pressure and temperature, particular emphasis will be sought in this regime, as they can unfold the physics of planetary interiors. The combination of different approaches (e.g., Density Functional Theory, Path Integral Monte Carlo, Quantum Monte Carlo, etc.) and comparison with available experimental results are critical to assess the validity of predictions from first principles. Therefore, benchmarking predictions of density functionals with more sophisticated theories is encouraged. This Special Issue covers all aspects of first principles calculations applied to minerals, with an emphasis in applications to planetary science, understanding basic physics at high pressure, numerical methods, and novel approaches.

Guest Editor

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About the Journal

Message from the Editor-in-Chief

Minerals welcomes submissions that report basic and applied research in mineralogy. Research areas of traditional interest are mineral deposits, mining, mineral processing and environmental mineralogy. The journal footprint also includes novel uses of elemental and isotopic analyses of minerals for petrology, geochronology and thermochronology, thermobarometry, ore genesis and sedimentary provenance. Contributions are encouraged in emerging research areas such as applications of quantitative mineralogy to the oil and gas, manufacturing, forensic science, climate change, geohazard and health sectors.

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Journal Rank:

JCR - Q2 (Mining and Mineral Processing) / CiteScore - Q1 (Geology)

Rapid Publication:

manuscripts are peer-reviewed and a first decision is provided to authors approximately 18 days after submission; acceptance to publication is undertaken in 2.5 days (median values for papers published in this journal in the second half of 2024).

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