Special Issue

First Principles Calculations of Minerals and Related Materials

Message from the Guest Editor

The aim of this Special Issue, "First Principles Calculations of Minerals and Related Materials", is to highlight the usefulness of first principles computational techniques to characterize the fundamental (structural, thermodynamical, elastic, optical, vibrational, surface, reactivity) properties of minerals. Both theoretical and joint experimental–theoretical works are welcome for this Issue, with special emphasis on (but not limited to) the study of the fundamental properties of minerals and closely related compounds, both at zero temperature and as a function of pressure and/or temperature. This includes the application of novel methodological approaches (new functionals, etc.), crystal structure prediction methods (USPEX, Calypso), the calculation of high-temperature and high-pressure phase diagrams of minerals, or the reliability of DFT calculations to include long-range interactions. Works dealing with the usefulness of alternative methods (molecular dynamics, Monte Carlo simulations, or multi-reference methods) are also welcome.

Guest Editor

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Deadline for manuscript submissions

closed (1 September 2021)

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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.

Editor-in-Chief

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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 18.2 days after submission; acceptance to publication is undertaken in 2.6 days (median values for papers published in this journal in the first half of 2025).

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