



minerals



an Open Access Journal by MDPI

First Principles Calculations of Minerals and Related Materials

Guest Editor:

Dr. Jordi Ibanez-Insa

Geosciences Barcelona
(GEO3BCN-CSIC), Lluís Sole i
Sabaris s/n, 08028 Barcelona,
Spain

Deadline for manuscript
submissions:

closed (1 September 2021)

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.



mdpi.com/si/39873

Special Issue



Editor-in-Chief

Prof. Dr. Leonid Dubrovinsky

Bayerisches Geoinstitut,
University Bayreuth, D-95440
Bayreuth, Germany

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.

Author Benefits

Open Access: free for readers, with article processing charges (APC) paid by authors or their institutions.

High Visibility: indexed within Scopus, SCIE (Web of Science), GeoRef, CaPlus / SciFinder, Inspec, Astrophysics Data System, AGRIS, and other databases.

Journal Rank: JCR - Q2 (*Mining & Mineral Processing*) / CiteScore - Q2 (*Geology*)

Contact Us

Minerals Editorial Office
MDPI, St. Alban-Anlage 66
4052 Basel, Switzerland

Tel: +41 61 683 77 34
www.mdpi.com

mdpi.com/journal/minerals
minerals@mdpi.com
[X@Minerals_MDPI/](https://twitter.com/Minerals_MDPI/)