Special Issue

Computational Methods in Mineralogy and Geochemistry

Message from the Guest Editor

Computational methods and virtual experiments are increasingly playing a main role in revealing the fundamental science underpinning complex geochemical phenomena and in predicting mineral structures, properties, formation and reactivity. In particular, during the past two decades, the rapid development of supercomputing facilities and of new algorithms exploiting these growing hardware capabilities has lead computational techniques to become a complementary tool to both interpret and direct experiments. Indeed, major advances in predicting and interpreting polymorphism, optical properties, surface reactivity, phase stability, nucleation pathways, dissolution and crystal growth mechanisms (to mention only a few) have been achieved through a variety of ab initio, classical, and semi-empirical methods that allow accessing accurate electronic and atomic scale information.

Guest Editor

Dr. Raffaella Demichelis

Curtin Institute for Computation, The Institute for Geoscience Research (TIGeR), and Department of Chemistry, Curtin University, Perth, WA 6845, Australia

Deadline for manuscript submissions

closed (15 February 2019)

Minerals

an Open Access Journal by MDPI

Impact Factor 2.2
CiteScore 4.4

mdpi.com/si/16849

Minerals
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
minerals@mdpi.com

mdpi.com/journal/minerals

Minerals

an Open Access Journal by MDPI

Impact Factor 2.2
CiteScore 4.4

mdpi.com/journal/minerals

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

Prof. Dr. Leonid Dubrovinsky
Bayerisches Geoinstitut, University Bayreuth, D-95440 Bayreuth, Germany

Author Benefits

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 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).

MDPI