Special Issue

Molecular Simulation of Mineral-Solution Interfaces

Message from the Guest Editor

With the dramatic supercomputing hardware and software progress over the last 10–20 years, the geochemical research community is becoming more and more interested in the application of computational molecular modeling techniques for the studies of minerals and mineral-solution interfaces in order to solve a wide variety of important geochemical, mineralogical, and environmental problems. We invite contributions to this Special Issue on all aspects of molecular simulation of mineral-solution interfaces using various modeling techniques from quantum ab initio, to classical force field based molecular dynamics (MD) and Monte Carlo (MC) methods, to mesoscale coarse grained simulations, etc. Contributions making direct links between atomistic computer simulations of mineral-solution interfaces and molecular scale experimental studies, such as synchrotron X-ray, neutron scattering, and other surface-sensitive techniques, are espeically encouraged.

Guest Editor

Dr. Andrey G. Kalinichev

Laboratoire SUBATECH, UMR 6457–Institut Mines-Télécom Atlantique, Université de Nantes, CNRS/IN2P3, 44307 Nantes, France

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

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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

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

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