Special Issue

Application of Advanced Quantum Chemistry in Mineral Flotation

Message from the Guest Editors

The efficient development and utilization of mineral resources requires the refinement of the mineral flotation process. Advanced quantum chemistry (including valence bond theory, coordination field theory, molecular orbital theory and density functional theory), as a precise science for studying the microstructure and change laws of substances at atomic and molecular levels, serves as a powerful tool for research on mineral flotation processes. This Special Issue aims to summarize recent progress in the research on advanced quantum chemistry and computational simulation methods for the mineral flotation process. Three sections will be covered: **Section 1:** Applications of advanced quantum chemistry in the study of flotation reagents. **Section 2:** Applications of density functional theory in the study of mineral crystal and surface and interface structure properties. **Section 3:** Applications of density functional theory in the study of mineral–reagent and mineral–mineral interface chemistry.

Guest Editors

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Deadline for manuscript submissions

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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:

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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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