



Computational Methods in Mineralogy and Geochemistry

Guest Editor:

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Message from the Guest Editor

Dear Colleagues,

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.

Dr. Raffaella Demichelis

Guest Editor





Editor-in-Chief

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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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