

Special Issue

Recent Advances in Molecular Modeling of Clay Minerals Interfaces

Message from the Guest Editors

Clays and clay minerals, a rich family of hydrous aluminosilicates, represent very useful materials for numerous applications in diverse industrial and environmental fields due to their low cost, natural availability, and ecofriendly character. Therefore, there is a paramount need to understand and predict the structure, physical properties, and reactivity of surfaces and interfaces of clay mineral particles at a molecular scale. To this end, molecular modelling studies play an important role. This Special Issue is focused on the most recent advances and achievements in molecular simulations of clay mineral surfaces and interfaces. Full papers, including reviews, covering the current trends and applications of a broad range of molecular simulation methods in this field are all welcome. The submission of papers addressing the topics listed below is particularly encouraged.

Guest Editors

Prof. Dr. Daniel Tunega

Dr. Edgar Galicia-Andrés

Dr. Peter Grancic

Deadline for manuscript submissions

closed (9 April 2021)



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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

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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).