Theoretical and Computational Mineral Physics

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Knowledge of crystallographic, chemical and physical properties of minerals is required to advance our understanding of the structure and dynamics of the Earth and planetary interiors. In the past decade, this has largely progressed based not only on experimental studies but also on theoretical and computational studies within the applications of various techniques, from first principles to empirical, from static calculations to molecular dynamics, and from atomistic to multi-scale models. This session will bring together the latest contributions related to computational studies of a wide range of mineral properties, including but not limited to structure, phase equilibria, thermodynamics, elasticity, diffusion, conductivity, transport properties, viscosity, etc. The scope of this session covers all studies of crystalline and amorphous materials within a broad range of compositions relevant in mineralogy. Through our presentations and discussions, we hope to create new paths for breakthroughs in future research directions within the field of computational mineralogy.