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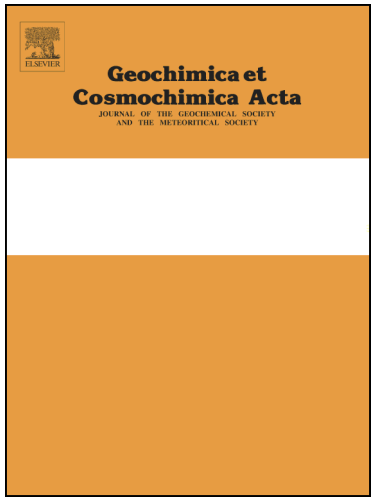

Trace element partitioning between silicate melts - a molecular dynamics approach

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Trace element partitioning between silicate melts - a molecular dynamics approach

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Abstract

Knowledge of trace element partition coefficients is crucial for our understanding of global element cycles. While a great number of experimental studies on mineral-melt partitioning have been performed in the past, the influence of melt structure on partitioning has mostly been considered empirically. This is mainly due to the lack of reliable structure models for typical melts at the relevant pressure and temperature conditions. Molecular dynamics simulations on the other hand may open a new window into this problem as they provide a unique approach to both structural and thermodynamic properties of minerals and melts. In this contribution, we employ first-principles and classical molecular dynamics simulations to (1) explore further a new approach to predict trace element partitioning between several silicate melts and (2) simultaneously investigate the structural controls of the observed partitioning. Specifically, we use a thermodynamic integration

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