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The Reduced Partition Function Ratios of K and Ca Isotopes in Feldspars: Insight from Deep Neural Network Potentials

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Feldspars are widely distributed in the crusts of the Earth, Moon, and terrestrial planets, which exhibit significant variations in chemical composition. These crustal variations result from diverse magma processes. The fractional crystallization history of feldspars, including alkali-feldspars and plagioclases, can be traced through the K and Ca isotopes compositions of the crusts, providing insights into terrestrial magma processes. Understanding the offset of K and Ca isotopes compositions during feldspar-related geochemical processes requires accurate equilibrium K and Ca isotope fractionation factors between feldspar and other phases. However, common feldspars exist as ternary solid solutions, exhibiting variations in their K, Ca, and Na contents, which may affect the equilibrium fractionation factors. First-principles methods have difficulties directly calculating the concentration effects influenced by variations in multiple components, leading to a current lack of equilibrium K and Ca isotope fractionation factors for feldspars.

In this study, we trained a deep neural network model using data from first-pricinples calculations to provide the potential energy and interatomic forces. The training set was initialized by performing first principles molecular dynamics calculations on feldspar supercells with varying compositions, and subsequently enhanced through active learning processes. The trained model shows a root mean square error of less than 5 meV/atom in potential energy and less than0.2 eV/Å in interatomic forces compared to first-principles data. We explored the concentration effect in feldspar supercells containing 208 atoms. We conducted substitutions at cation sites (K/Na/Ca) to simulate different concentrations and tested the effects of unequal occupation by swapping K/Na/Ca and tetrahedral sites (Al/Si) within each concentration.The reduced partition function ratios of K and Ca isotopes of each concentration were averaged across the values of these occupation scenarios, weighted by their free energies. Our results provide a quantitative approach for estimating the effects of K and Ca isotopes on feldspar-related processes during the evolution of melts.