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Estimates of lithium isotope fractionation factors using density functional theory: Applicaitons to LCT pegmatite systems

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Lithium is a fluid-mobile and incompatible element, that is enriched in highly differentiated felsic systems, particularly in lithium-cesium-tantalum (LCT) pegmatites. While Li isotope fractionation has often been considered negligible at magmatic temperatures, recent studies reveal variations of Li isotope (δ^7Li) exceeding 10‰ in pegmatites, highlighting the need for a quantitative understanding of the controlling mechanisms [1]. A key limitation lies in the absence of reliable fractionation factors for silicate melts, likely due to the complexities in melt structures, composition, and dynamics.

To address this knowledge gap, *ab initio* molecular dynamics and density functional theory calculation were used to compute equilibrium lithium isotope fractionation factors among Li-bearing minerals, hydrothermal fluids, and felsic melts. The results show that the composition, water content, and halogen (F/Cl) significantly influence Li isotope partitioning by modifying Li-O bond length, coordination environments, and polyhedral structure.

At the deposit scale, compilation of δ^7Li data from LCT pegmatites and granites worldwide shows that the largest isotope fractionation occurs prior to lithium mineralization. To investigate the underlying mechanisms, we developed numerical models incorporating fractional crystallization, fluid exsolution, melt-melt immiscibility, and further kinetic isotope effects associated with rapid crystal growth and diffusion. The results demonstrate that fractional crystallization and melt-melt immiscibility induce δ^7Li variations of up to ~3‰, whereas fluid exsolution can drive δ^7Li shifts exceeding 10‰ in residual melts at magmatic temperatures. Additionally, kinetic induced isotope fractionation further contributes to shifts in δ^7Li up to 15‰. These findings suggest that the pronounced Li isotope variations (>10‰) observed in pegmatite deposits, such as Jiajika, Tin Mountain, and Qinghe, are dominantly controlled by fluid exsolution and kinetic effects, providing new insights into the lithium isotopic evolution during petrogenesis and mineralization of pegmatite systems.

[1] Lei X.-F., Romer R. L., Glodny J. and Jiang S.-Y. (2023). *Geology* 51, 581–585.