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Boron isotope fractionation between magmatic fluids and melts determined by machine learning potentials

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Boron isotopes are widely used to study geochemical cycles and interactions between magmas, minerals, and aqueous fluids. The wide range of observed B isotope compositions, the high mobility of B in hydrothermal and magmatic fluids and the frequent occurrence of B-bearing minerals such as tourmaline in ore deposits make boron an important geochemical tracer for ore-forming processes. While B isotope fractionation between different minerals and between minerals and fluids has been studied in experiments and by computer simulations, the fractionation between silicate melts and exsolved aqueous fluids, e.g., at the magmatic-hydrothermal transition, is largely unknown. As the major B isotope fractionation occurs between B in planar trigonal (BO_3) and tetrahedral (BO_4) coordination, the speciation of B in the melt and in the coexisting fluid needs to be studied and understood.

In this work we use molecular dynamics simulations combined with a developed machine-learning force field (MLFF) to investigate the structure of various silicate melts and aqueous fluids, and in particular the molecular structure of BO_3 and BO_4 complexes in these phases. The MLFF trained on electronic structure calculations and snapshots from *ab-initio* molecular dynamics (AIMD) simulations using the DeepMD approach [1], accurately reproduce the structural, dynamical and vibrational properties of these systems. Using this methodology, we estimate $^{11}B/^{10}B$ equilibrium isotope fractionation factors through several computational approaches [2]. Additionally, we examine the effect of Na_2O (NaCl) content on the $^{11}B/^{10}B$ equilibrium isotope fractionation. Finally, we compare our results with previous experimental and simulation data.

[1] Wang et al. (2018) *Comput. Phys. Commun.* 228, 178-184.

[2] Pinilla et al. (2015) *Geochim. Cosmochim. Acta* 163, 126-169.