structures within a given mineral suggests that the isotopic signatures of soil (oxy) hydroxide could be heterogeneous.

Density functional and correlated molecular orbital calculations (MP2) are carried out on $B(OH)_3 \cdot nH_2O$ clusters (n = 0, 6, 32) and $B(OH)_4 nH_2O$ (n = 0, 8, 11, 32) to estimate the equilibrium distribution of ^{10}B and ^{11}B isotopes between boric acid and borate in aqueous solution. For the large 32-water clusters, multiple conformations are generated from ab initio molecular dynamics simulations to account for the effect of solvent fluctuations on the isotopic fractionation. We provide an extrapolated value of the equilibrium constant á$_{34}$ for the isotope exchange reaction $^{10}B(OH)_3(aq) + {}^{10}B(OH)_4(aq) = {}^{11}B(OH)_3(aq) + {}^{11}B(OH)_4\ (aq)$ of 1.026—1.028 near the MP2 complete basis set limit with 32 explicit waters of solvation. With some exchange-correlation functionals we find potentially important contributions from a tetrahedral neutral $B(OH)_3 \cdot H_2O$ Lewis acid–base complex. The extrapolations presented here suggest that DFT calculations give a value for 103lná$_{34}$ about 15 % higher than the MP2 calculations.

Interaction of earthquakes and slow slip: Insights from fault models governed by lab-derived friction laws

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California Institute of Technology, Pasadena, CA, USA

Motion of plates in the Earth crust is accomodated through fault slip. That includes both fast events (earthquakes) and slow relative motion, as evidenced by seismic and geodetic observations. We study mechanics and physics of earthquakes using a unique simulation approach that reproduces both earthquakes and slow slip, with full inclusion of inertial effects during simulated earthquakes, in the context of a 3D fault model. The approach incorporates laboratory-derived rate and state friction laws, including the effects of shear heating during rapid, seismic slip, involves slow, tectonic-like loading, resolves all stages of seismic and aseismic slip, and results in realistic rupture speeds, slip velocities, and stress drops. Our simulations show that a number of observed earthquake phenomena can be explained by interaction of earthquakes and slow slip, including transition to intersonic rupture speeds during earthquakes, peculiar properties of small repeating earthquakes, and complex spatio-temporal patterns of earthquake sequences.