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Molecular Paleoclimatology: Quantum Chemistry and the History of the Earth's Atmosphere

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The history of the composition of the Earth's atmosphere is one of the most important problems of our time. As the human race considers the possibility of planetary engineering to mitigate the potential effects of CO_2-induced global warming, clearer insight into the history of atmospheric PCO_2 and global temperature is required. For example, if PCO_2 values were 20 times higher at times in the geologic past, it may be premature to worry about anthropogenic increases in PCO_2 a factor of two above Pleistocene-Holocene values, which are anomalously low from the point of view of geologic history. Two major techniques for determining the history of atmospheric PCO_2 are the chemically based. The first depends on the isotopic composition of carbon incorporated into soil minerals during their growth. The second depends on the isotopic composition of boron incorporated into marine minerals during precipitation. Both methods depend crucially on knowing the equilibrium constant for isotope exchange between minerals, aqueous, and gas phases. There are major uncertainties in these equilibrium constants which strongly affect geochemical estimation of the history of PCO_2 in Earth's atmosphere. Here, I describe how quantum chemistry techniques can be used to reduce this uncertainty and make more reliable estimates of PCO_2 values.

Ab initio molecular dynamics and quantum chemistry techniques are used to calculate the structure, vibrational frequencies, and carbon-isotope fractionation factors of the carbon dioxide component [CO_2(m)] of soil (oxy)hydroxide minerals goethite, diaspore, and gibbsite. We have identified two possible pathways of incorporation of CO_2(m) into (oxy)hydroxide crystal structures: one in which the C^{4+} substitutes for four H^+ [$CO_2(m)_A$] and another in which C^{4+} substitutes for (Al^{3+},Fe^{3+})+H^+ [$CO_2(m)_B$]. Calculations of isotope fractionation factors give large differences between the two structures, with the $CO_2(m)_A$ being isotopically lighter than $CO_2(m)_B$ by≈10 per mil in the case of gibbsite and nearly 20 per mil in the case of goethite. The reduced partition function ratio of $CO_2(m)_B$ structure in goethite differs from CO_2(g) by<1 per mil. The predicted fractionation for gibbsite is>10 per mil higher, close to those measured for calcite and aragonite. The surprisingly large difference in the carbon-isotope fractionation factor between the $CO_2(m)_A$ and $CO_2(m)_B$

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 $\acute{a}_{34}$ 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 $10^3 \ln \acute{a}_{34}$ 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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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.

Numerical simulations of short-timescale geomagnetic field variations

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Numerical modeling of the convection in the Earth's liquid outer core has succeeded in simulating generation of a dipole-dominated magnetic field and its intermittent polarity reversals. However, previous models have used unrealistically high viscosity for the core fluid because of computational difficulty to resolve small-scale turbulence that would otherwise happen. It is still an open question whether lower-viscosity Earth-type dynamo models can simulate the geomagnetic field and its time varia-