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Formation and Isotopic Evolution of Earth's Earliest Oceans

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How Earth's earliest oceans formed, and whether their hydrogen and oxygen isotope composition has remained constant since the Hadean, are two long-standing and fundamental questions in Earth and planetary sciences. Although numerous studies have debated the secular evolution of seawater isotopes [1, 2], progress has been limited by the absence of quantitative constraints on the isotopic composition of Earth's earliest oceans —the baseline from which all subsequent evolution proceeds.

Here we employ machine learning–accelerated path-integral molecular dynamics to quantify equilibrium hydrogen and oxygen isotope fractionation between silicate melt and coexisting vapor at pressures and temperatures relevant to magma ocean degassing. By integrating these fractionation factors into thermal evolution models, we derive the first quantitative estimates of the hydrogen and oxygen isotope composition of Earth's earliest oceans.

Our results show that Earth's earliest oceans formed through magma ocean degassing followed by atmospheric condensation during planetary cooling. These oceans likely exhibited elevated $\delta^{18}O$ values and δD values comparable to or more negative than those of Archean [3, 4] and modern seawater (~0‰). We further demonstrate that ocean isotope compositions have evolved since ~4.5 Ga rather than remaining static, providing a dynamic framework that reconciles previously conflicting hydrogen and oxygen isotope records from the Archean to the present [3-6]. In addition, we identify a major transition in surface processes, from early serpentinization-dominated alteration of an ultramafic crust to a weathering-dominated surface regime. This shift links the evolution of ocean isotopes to fundamental changes in geodynamics, crustal composition, and surface environment.

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