

## Isotope clues for the early differentiation of the Earth

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The first 500 million years of Earth's history were marked by violent events that resulted in a massive differentiation of the Earth, including the formation of a metal core, of a crust and of an atmosphere. These events seem to have taken place relatively rapidly after the Earth's accretion and could even be coupled to each other. Our views regarding these events have rapidly evolved over the past few years, with the several revisions of the timing of these events and more accurate description of the processes involved.

One would expect that the core-formation that explains the  $^{182}\text{Hf}$ - $^{182}\text{W}$  systematics and magma ocean crystallization that explains the  $^{146}\text{Sm}$ - $^{142}\text{Nd}$  should be almost synchronous. However, in the case of the Moon, the nominal  $^{146}\text{Sm}$ - $^{142}\text{Nd}$  age is at least 100 Ma younger than the accretion age while for Mars it is at least 20 Ma younger. The crystallization time scale for magma ocean is about 10 Ma for an Earth-sized object, thus there seems to be a discrepancy between the Sm-Nd chronology and the time scales based on dynamical models, except for the Earth. Several explanations have been put forward to explain this observation, including the effect of mixing or contamination of magmas or the cumulative overturn that should have taken place after magma ocean crystallization. Yet, it is very difficult to envisage a process that would result in planetary scale isotope equilibration, producing an Sm-Nd 'mantle isochron'. It can be therefore argued that some subsequent fractionation related to magmatic processes could have altered the slope of these mantle isochrons, whereby depleted component would be further depleted, while enriched component would be further enriched. Such a process would alleviate the problem of having a late process of isotope equilibration.

## Molecular dynamics simulations of brine-clay interfaces: Implications for CO<sub>2</sub> storage in saline aquifers

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Storage of fossil fuel-derived CO<sub>2</sub> in deep geologic formations could contribute up to 40 % of the emissions reductions required to stabilize global temperatures over the next century [1]. This approach, known as carbon capture and storage (CCS), involves injecting supercritical CO<sub>2</sub> into suitable formations under clay caprock, such as saline aquifers or depleted hydrocarbon reservoirs. Our ability to predict, and eventually control, the behavior of CO<sub>2</sub> in these porous media will require a detailed understanding of mineral-water-CO<sub>2</sub> interfacial phenomena in the caprock such as adsorption, interfacial tension, solid nucleation and growth, mass transfer through and along interfaces, and the forces between adjacent interfaces [2-4].

Insights into the nanoscale behavior of water near mineral surfaces can be readily obtained by molecular dynamics (MD) simulation. However, few previous studies have simulated water films sufficiently thick to probe the full transition from interfacial water to bulk liquid water [5, 6] or ionic concentrations that approach those in saline aquifers [6-8]. We used tested clay-water MD simulation methodologies [9] to study Na-Ca-Cl brines with ionic concentrations of 0.2 to 1.6 mol<sub>c</sub> dm<sup>-3</sup> in a 5.8 nm pore between smectite clay surfaces. These simulations reveal how brine concentration influences cation exchange selectivity, the shape of the electrical double layer, and water and solute diffusion near clay surfaces. We also report simulations of CO<sub>2</sub>-saturated brines in smectite nanopores that evince how brine concentration affects adsorption and diffusion of dissolved CO<sub>2</sub> near clay surfaces.

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