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# CO<sub>2</sub> Solvation in Molten Silicates and Carbonates From First-Principles: From the Earth Mantle to Fuel Cells

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## Résumé

Although the carbon content of the Earth mantle is very low, carbonated magmas play an important role in the mantle dynamics. Indeed, while carbonated magmas are very scarce at the Earth surface, they are the main liquid component at the onset of melting. These carbonated magmas have a much lower viscosity than typical molten silicates and play a crucial role in the chemical differentiation of the mantle and CO<sub>2</sub> degassing. Understanding the chemical speciation of CO<sub>2</sub> in these liquids is key to our understanding of their dynamical and thermodynamical properties. We will present first-principle molecular dynamics simulations of CO<sub>2</sub> dissolved in some model natural silicates to investigate this speciation. The end member of these liquids is pure molten carbonate. Some are also found in the Earth mantle but they have another application as electrolyte in molten carbonate fuel cells. Among the peculiar properties of molten carbonates is their ability to dissolve CO<sub>2</sub> at least two orders of magnitude better than other molten salts. First-principle molecular dynamics simulations of CO<sub>2</sub> in molten carbonates has revealed the appearance of a new species, the pyrocarbonate anion, that plays an intermediate role for CO<sub>2</sub> transport through a Grotthuss-like mechanism. After presenting these results, we will discuss their implication for the use of molten carbonates as electrolyte for the electroreduction of CO<sub>2</sub>.

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