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INVITED SPEAKER: From carbon speciation to transport properties of carbon rich liquids of the upper mantle from molecular dynamics simulations

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Abstract content
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Although the carbon content of the mantle is very low it plays an important role in the mantle dynamics. In the upper mantle, carbon has mainly the form of carbonates and at the onset of fusion the molten fraction of the mantle are carbonate rich liquids or even molten carbonates. Upon reaching shallower depths, the liquid formed gets richer in silicate content. These carbonate rich liquids have a very low viscosity and low density and thus impact the mantle dynamics. They are also characterized by high ionic conductivity, about four order of magnitude larger than that of molten silicates. This property led to evidence of the presence of these liquids at a few hundred kilometers depth through magnetotelluric experiments.

These properties are directly linked to the microscopic structure of these liquids. Here, we employ two levels of molecular dynamics simulations, first-principle molecular dynamics and classical molecular dynamics, to identify the microscopic structures of carbonate rich fluids and predict their density and transport properties. Some consequences on the mantle geophysics will then be discussed.

Furthermore, we show that molten carbonates can solvate CO₂ and we found a new mechanism for CO₂ transport through fast O²⁻ exchange. This may have implication for CO₂ capture and storage.

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