The effects of water on silicate melts by molecular dynamics simulations

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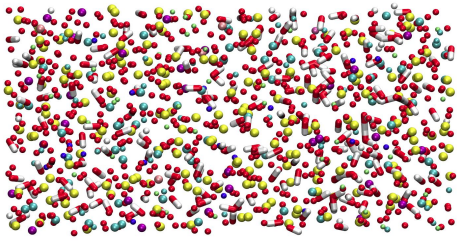
Water represents ~ 0,5% of the Earth's mass, the major part (the oceans contribute only 0,023%) of it being stored in mantle's silicates. However a tiny amount of water may have a huge impact on the transport properties of silicate melts [1], the melting temperature of mantle minerals and plate tectonics [2]. Among others in case of volcanic eruption, the exsolvation of water may cause a high increase in the viscosity of the ascending magma, leading eventually to catastrophic pyroclastic flows.

Although experimental data on the properties of hydrous silicate melts are growing, it is still difficult to investigate *in situ* the properties of such systems at liquidus temperature. That is why, as a theoretical guide, we use classical molecular dynamics simulations to model silicate liquids at mantle conditions. Lately we have developed a force field to describe the properties of dry silicate melts [3] of various compositions. We present here the last development of this force field to account for the incorporation of water. We will illustrate the heuristicity of this model potential with the examples of basaltic (MORB) and andesitic melts. We discuss how water dissolves in the melt as a function of pressure and temperature and we investigate the effects of water on some key properties, such as the density, the viscosity or the electrical conductivity.



Snapshot of a hydrous silicate (MORB)

[1] P. Richet *et al*, *Chem. Geol.* 128.1 (1996): 185-197. [2] M. Hirschman, D. Kohlstedt, *Physics Today* **65**, 3, 40 (2012); doi: http://dx.doi.org/10.1063/PT.3.1476 [3] T. Dufils *et al*, *Chem. Geol.* (2016), http://dx.doi.org/10.1016/j.chemgeo.2016.06.030