Influence of water on the critical point of silica

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Silica is a major rock forming material in our Solar System. The formation of rocky bodies depends on accretion and giant impacts, which often produce silicate fluids. The most recent theory of Giant Impact for the Moon formation implies in the formation of a synesthia in the aftermath of the impact. In this scenario, a hot silicate atmosphere would have formed and if there would be an ocean, it would be vaporized as well together with the material. Hence, placing the critical point of the SiO_2 – H_2O binary system has implications for understanding the conditions at the formation of the Earth-Moon system, but also for other geological scenarios such as subducction zones.
Here we study the effect of H_2O on the supercritical and subcritical properties of SiO_2 fluids from first-principles molecular dynamics modeling We use cristobalite with 72 SiO_2 units as a starting condition. The material was heated up to 3000K and 4000K and then 8 and 16 units of H_2O were added to the system. We show the variation of the spinodal lines and we discuss the polymerization of the fluids. We analyze the chemical speciation and the vaporizaiton.

Mots-Clés : critical point, silica, water, impact, ab initio, supercritical fluid

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