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The behaviour of MgO in a giant impact setting

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The Earth-Moon system and its formation is a topic of great scientific interest, and great debate over the past decades. The giant impact hypothesis is the currently accepted model to explain the formation of our moon. Accordingly, a mars-sized impactor collides with the proto-earth. This giant impact vaporized a significant portion of the impactor and the proto-earth, creating a large accretionary disk from which the moon subsequently formed. Currently, there is a large effort to build reliable thermodynamic descriptors for the building materials of the two bodies involved in the impact. Understanding the behavior of major rock-forming minerals under these extreme conditions is vital for increasing the accuracy of these models.

Magnesium oxide, MgO, is one of the fundamental building blocks for rocky planets. It is an archetype material of ionic solids and a well-known refractory material. Because of its relevance it has been studied extensively; experimental and theoretical results have been produced up to pressures of 800 GPa and temperatures reaching 20000 K. These pressure and temperature regions are of great interest for the planetary sciences, studying planetary interiors. The transformation of the face-centered B1 phase to the body-centered B2 phase and the associated melting curve have been modelled numerous times. In contrast, we know very little of the liquid behaviour of MgO under pressure, let alone at the low pressures found in accretionary disks.

Here we investigate the low-density high-temperature regime characteristic of after-shock isentropic release. We explore the subcritical and the supercritical regimes of MgO using ab initio molecular dynamics. We determine the position of the critical point and examine the structural and transport properties in the sub- and supercritical regimes. We find an elevated critical temperature in comparison with previously studied magnesium-silicates, in agreement to the refractory nature of MgO. Furthermore, we provide insight into the speciation of liquid MgO and the liquid-gas separation. We see a shift in Mg-O speciation towards lower degrees of coordination as the temperature is increased from 4000K to 10000K. This shift in speciation is less pronounced at higher densities. The majority of the chemical species forming the incipient gas phase consist of isolated Mg and O ions and some MgO and O_2.

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