Supercritical and subcritical regimes of MgO

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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 trying to explain the formation of our moon. However, many details about the parameters of the impact and of the impactor are missing. Currently there is a large effort to build reliable thermodynamic descriptors for the building materials of the two bodies involved in the impact. MgO is one of the major components of the bulk earth and moon. Here we investigate the subcritical and supercritical regimes of MgO using ab initio molecular dynamics. We find the critical temperature between 6500 and 7000K, which is likely related to its refractory properties. We build the Hugoniot equation of states and characterize MgO under extreme shock. Then 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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