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The melting curve of $MgSiO_3$ perovskite from ab initio molecular dynamics

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Despite its importance in understanding such things as the crystallisation of the Earth's mantle from a magma ocean or the existence of melt in the current mantle (i.e. in ULVZs), the melting temperature of the lower mantle phase $MgSiO_3$ perovskite is poorly known. Estimates of its melting temperature at the core-mantle-boundary range from 5400 K to over 8000 K. We have used, therefore, ab initio molecular dynamics simulations to predict its melting temperature throughout the Earth's mantle. In particular we have used the coexistence method where both solid and melted perovskite exist in the same super-cell. For these simulations we used 900 atoms (a 3x3x5 super-cell) with atoms in one half of the super-cell melted and the other half solid. The melt side was generated by increasing the temperature to very high values while keeping atoms in the solid side fixed. Once melted we gradually lowered the temperature to the desired temperature and thermalisation was then turned off. The system was then allowed to evolve in an NVE simulation using DFT forces calculated within the LDA. Those systems which were too hot melted within 10 ps. Those which didn't remained with both solid and melt coexisting in the super-cell for over 25 ps. These where assumed to be either on the melting curve of just below it. Our results agree well with the higher temperature melting curves found experimentally, and we predict a melting temperature of about 6500 K at the core-mantle boundary.