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The melting curve of MgSiO3 perovskite from ab initio molecular dynamics using the coexistience method

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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, the melting temperature of the lower mantle phase MgSiO3 perovskite is poorly know. 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 using the coexistence method. We used 900 atoms (a 3x3x5 super-cell) with atoms in one half of the super-cell melted and the other half solid. Both halves are thermalised to the desired temperature individually. We then turned off the thermalisation and allowed the system to evolve in an NVE simulation, using DFT forces calculated within the GGA. 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. We will also present results on simulating the melting temperature of the MgO-MgSiO3 binary.