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Post-perovskite $MgCO_3$ phase at pressures up to 800 GPa JONES TSZ-KAI WAN, Department of Physics, The Chinese University of Hong Kong — The high-pressure phases of magnesite ($MgCO_3$) are investigated by variable cell first-principles molecular dynamics simulations. At pressures compatible to lower mantle conditions ($\sim$120 GPa), the carbon atoms are surrounded by 4 oxygen atoms, which is consistent with the work of Skorodumova et al. (2005). Perovskite phase is observed at pressures greater than 300 GPa, but its stability is still subject to further studies. Stable post-perovskite structure is observed at pressures up to 800 GPa, and is found to be more stable than the perovskite phase. The results may bring important implications to interior models of giant planets, which may lead to a better understanding in giant planets physics.

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