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**First-principles study of $MgSiO_3$ at core-mantle boundary conditions** SIU-CHUNG SUNG, The Chinese University of Hong Kong, JONES TSZ-KAI WAN — Perovskite $MgSiO_3$ is an important mineral in geoscience studies. It plays a crucial role in the understanding of geophysical and geochemical activities taken place in the Earth's interior. In this talk, we report our recent work on First-principles molecular dynamics (FPMD) simulations of solid $MgSiO_3$ perovskite and post-perovskite, and molten $MgSiO_3$ at core-mantle boundary (CMB) conditions. The equations of state are determined at pressures up to 200 GPa and temperatures up to 6000K. The post-perovskite phase is found to be favoured over the perovskite at pressures above 102 GPa at zero temperature. Melting of $MgSiO_3$ has been observed by heating both perovskite and post-perovskite at high temperatures ($\sim$6000 K). The melting curve and electronic structures of solid and molten $MgSiO_3$ are also presented. Our simulated results thus provide useful constraints on structure and phase stability of $MgSiO_3$, which is the key to the understanding of deep-earth phenomena, such as the D$''$ discontinuity and seismic anisotropies in D$''$ layer. More importantly, the phase transformation of $MgSiO_3$ studied in this work provides insights into other aspects of geosciences like chemical heterogeneity and mantle convection, which may lead to a better model of the Earth's evolution.

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