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Thermodynamic properties of $MgSiO_3$ majorite and phase transitions near 660-km depth in $MgSiO_3$ and Mg_2SiO_4: a first principles study[1] YONGGANG YU, Virginia Tech, RENATA WENTZCOVITCH, U. Minnesota, VICTOR VINOGRAD, U. Frankfurt, ROSS ANGEL, Virginia Tech — Thermodynamic properties of $MgSiO_3$ tetragonal majorite have been calculated at high P-T within the quasiharmonic approximation based on DFT using both LDA and GGA. The LDA results compare exceptionally well with measured thermodynamic properties. A classical Monte Carlo simulation based on a cluster expansion method demonstrates that disorder between Mg and Si in the octahedral sites in majorite does not occur below 3600 K within 30 GPa. The calculated phase boundaries between majorite (mj), perovskite (pv), and ilmenite (il) $MgSiO_3$ agree much better with experiments by using GGA than by LDA. The Clapeyron slopes (CS) predicted by GGA and LDA are close to each other: 0.9 – 1.7 MPa/K for mj-pv, 6.9 – 7.9 MPa/K for mj-il, and -7 – -3 MPa/K for il-pv transition. The triple point predicted by GGA is at 21.8 ± 1 GPa and 1840 ± 200 K which is $\sim$400 K lower than most experiments. Our calculations also reveal that wadsleyite decomposes to an assemblage of majorite plus periclase above 2280 K with a large negative CS (-22 – -12 MPa/K) and that ringwoodite decomposes to ilmenite plus periclase below 1400 K (1.2 MPa/K). The geophysical implications to mantle convection and the composition of the Earth's transition zone will also be discussed.

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