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**First principles studies on several major phase transitions in Earth upper mantle** YONGGANG YU, Univ. of Minneosta, ZHONGQING WU, U of Minneosta, RENATA WENTZCOVITCH, U of Minnesota, CHEMICAL ENGINEERING AND MATERIALS SCIENCE TEAM — First principles quasi-harmonic free energy calculations have been conducted to study several important phase transitions in mantle minerals with compositions  $\text{Mg}_2\text{SiO}_4$  and  $\text{MgSiO}_3$  under realistic Earth's mantle conditions. We find encouraging and similar level of agreement with experiments for thermodynamic and vibrational properties and phase transition boundaries in all cases where comparisons between results and data are possible. We also find systematic trends: 1) equations of state and thermodynamic properties of single crystalline phases are best described by the LDA; 2) phase boundaries are bracketed by LDA and GGA results, with GGA offering the upper bound transition pressure and being somewhat closer to the experimental ones. A summary of these results is offered for forsterite, wadsleite, ringwoodite, periclase, perovskite, post-perovskite, low clino-, and high clino-enstatite, and garnet, as well as phase transitions between them. In overall these results can supplement high-PT experimental data on these minerals. (Research supported by NSF/EAR 013533, 0230319, 0635990, and NSF/ITR 0428774 (VLab), and Minnesota Supercomputing Institute.)

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