s11.m2.o5 **Simulating Phase Transitions and Thermoelasticity of Mantle Minerals.** A.R. Oganov, J.P. Brodholt, G.D. Price, *University College London, Gower St., London WC1E 6BT, U.K.*
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Using a variety of computer simulation methods, ranging from *ab initio* density functional to semi-classical calculations, from static to lattice-dynamical and molecular dynamics approaches, we consider phase transitions in the Al_2SiO_5 system[1,2] (phase diagram, hypothetical V_3O_5- and pseudobrookite-like phases in the Mantle, metastable pressure-induced isosymmetric, incommensurate, and amorphisation transformations of andalusite and sillimanite) and the major Earth-forming mineral, $MgSiO_3$-perovskite[3] (transition from the orthorhombic to tetragonal and cubic phases, diffusion and ionic conductivity). We also discuss thermoelastic properties of $MgSiO_3$-perovskite at the Lower Mantle conditions. Insights at the microscopic level as well as some global geophysical implications of our results will be presented.

We develop a new view on phase transitions, based on the symmetry and topology changes upon the transition. From this viewpoint, phase transitions can be divided into local, or evolutionary phase transitions (the transition involves minimum changes in symmetry and topology, necessary to maintain crystal's stability. At the onset of an intrinsic instability, the system goes into the nearest local free energy minimum, which is not necessarily the global minimum), and global phase transitions (the new phase always corresponds to the global free energy minimum, and there is no structural relation between the old and new phases). The local transitions can be further classified according to the degree of symmetry breaking: isosymmetric > group-subgroup relations>incommensurate transitions > pressure-induced amorphisation. Our classification naturally incorporates traditional notions of first/second order, reconstructive/displacive, order-disorder transformations. Examples from our recent theoretical works on Al_2SiO_5[1,2], $MgSiO_3$[3], and SiO_2[4] include all major types of phase transitions.

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