Molecular dynamics simulation of aluminous perovskite

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We have been investigating the physical properties of aluminous perovskite (Mg, Al)(Al, Si)O3 through molecular dynamics (MD) method. The solid solution was made by substituting adjacent pairs of (Mg ion + Si ion) in MgSiO3 perovskite with Al ions, so as to satisfy the local charge balance. The values of the unit-cell parameters, volume, and enthalpy are comparable with those for the solid solution in which Al ions are randomly distributed. The characteristics such that Al2O3 enriched perovskite is more compressible than aluminum free perovskite are applicable, regardless of the pattern of the distribution of Al ions in the crystal.