

High-Pressure Phase Transitions in AlPO_4 from First-Principles

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Based on first-principles density functional theory calculations, we predicted a ferroelastic transition in AlPO_4 between stishovite-like and $m\text{-CaCl}_2$ phases by confirming the energetic stability of stishovite-like phase and witnessing a pressure-induced phenomena of symmetry-breaking spontaneous strain, and furthermore, we established a new pressure-induced phase transition sequence for AlPO_4 up to 100 GPa at 0 K as follow: berlinite to moganite, to AlVO_4 , to $P2_1/c$, to CrVO_4 , to stishovite-like, and to $m\text{-CaCl}_2$ phase, with the corresponding transition pressure 4.1, 5.0, 7.0, 7.3, 31.9 and 46.4 GPa, respectively. For all these phases, equation of state parameters are reported. This transition sequence largely revises the previous one based on in-situ cold-compression experiments, by incorporating four new phases, moganite, AlVO_4 , the $P2_1/c$, and stishovite-like, the former three of which were synthesized by our recent quench experiments and are theoretically investigated here for the first time. This newly-established phase transition sequence would serve as a model case because it is the most detailed one among all the berlinite-type ABO_4 compounds to date. This study would also provide deep insight into the polymorphism behavior of SiO_2 because of some instructive dissimilarities discerned between these two isoelectronic compounds, such as that all the mixed-coordinated phases in AlPO_4 exceptionally lack counterparts in SiO_2 , and that moganite is stable after quartz phase in AlPO_4 but metastable in SiO_2 .

Keywords: AlPO_4 , SiO_2 , phase transitions, high-pressure, first-principles, equation of state