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Phase transitions in Zn_2SiO_4: first-principles study

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Recent experimental study (Liu et al., PCM, 40, 467, 2013) suggested that high-pressure phases of III and IV in Zn_2SiO_4 could be retrograde phases transformed during decompression. In order to check stabilities of these phases under pressure, and to find original high-pressure phases, density functional theory total energy calculations of 12 phases at 0 K have been conducted.

Three pressure-induced "phase transitions" during structural optimization were observed: phase II to spinel structure, phase III to a new high-pressure phase, and phase IV to Na_2SO_4 III-type structure. Phase III, having tetrahedral olivine structure, exhibited extraordinary high compressibility, which is due to large volume reductions in vacant octahedral sites corresponding M1 and M2 sites in olivine structure. Calculated enthalpies of the phases at 0 K confirmed that phase III and IV are not stable at any pressure. It also suggested that Na_2SO_4 III and II phases will be stable phases replacing phase III and IV, respectively.

Keywords: Zn2SiO4, phase transition, high pressure phase, first-principles, transition mechanism