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New high-pressure phase relations in $CaSnO_3$

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ABSTRACT

High-pressure phase stabilities of the $CaSnO_3$ system were investigated using density functional theory static lattice energy calculations. We have identified six phase changes in this system: perovskite-post-perovskite, post-perovskite-B2+cotunnite in $CaSiO_3$, B1-B2 in CaO, cassiterite-pyrite, pyrite-orthorhombic-I, and orthorhombic-I-cotunnite in SnO_2. Our results demonstrate a new high-pressure phase sequence of perovskite → post-perovskite → B2 + cotunnite. The post-perovskite transformation occurs at ~12 GPa with ~2.5% volume reduction and then it decomposes into the oxide mixture of B2 CaO and cotunnite SnO_2 at ~70 GPa with 8.1% volume reduction. The results also predict a few percent bulk velocity variations across these phase changes.

Keywords: $CaSnO_3$, perovskite, post-perovskite, density functional calculation