

Abstract Submitted
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Potentially novel ultrahigh pressure form of ABX₃-type compounds¹ KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, MSI and CEMS, University of Minnesota — By means of first-principles computations we have identified two new dynamically stable structures that are candidate ultra-high pressure forms of ABX₃-type compounds. To our knowledge, they have not been experimentally observed yet. They are produced by metastable pressure-induced transformations in *Cmcm* NaMgF₃, a post-perovskite phase. The first transition to a *Pmcn* structure is related to a soft phonon mode in post-perovskite. The second one is a regular enthalpically driven transition from *Pmcn* to a *P6₃/mmc* structure. In NaMgF₃ these phases are metastable with respect to the dissociation into CsCl-type NaF and cotunnite-type MgF₂. However, the *Pmcn* phase might be observed at low temperatures. We have also identified a candidate post-perovskite material that prefers the *Pmcn* phase over the dissociation into AX- and BX₂-type solids.

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