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Post-perovskite transition in $NaMgF_3$ JOHN PARISE, Department of Earth and Space Science, SUNY-Stony Brook, NY 11794-2100, USA, KOICHIRO UMEMOTO, RENATA WENTZCOVITCH, Department of Chemical Engineering and Materials Science and Minnesota Supercomputing Institute, Univesity of Minnesota, DONALD WEIDNER, Department of Earth and Space Science, SUNY-Stony Brook, NY 11794-2100, USA — We have investigated through first principles computations the pressure-induced behavior of $NaMgF_3$. It has the same Pbnm perovskite structure as $MgSiO_3$, the major lower mantle phase. Likewise $MgSiO_3$ it displays the same post-perovskite transition. Static LDA calculations indicate this transition should occur shortly after 18 GPa and then decompose into NaF and MgF_2 above 40 GPa. Phonon dispersions and elastic moduli of the post-perovskite phase confirm its vibrational/mechanical stability. The existence of a post-perovskite transition at low pressures in this material makes possible experimental studies of this uncommon structure in a more easily accessible pressure range. Research supported by NSF/EAR 013533 (COMPRES), 0230319, and NSF/ITR 0428774 (VLab).

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