# High-Pressure Phase Transitions Beyond Post-Perovskite in Neighborite, $NaMgF_3$

R. Dutta[1*], E. Greenberg[2], V. B. Prakapenka[2] and T. S. Duffy[1]

[1]Department of Geosciences, Princeton University, NJ 08544, USA.
[2]Center for Advanced Radiation Sources, University of Chicago, Chicago, IL 60637, USA.

**Abstract**

The high-pressure behavior of neighborite, $NaMgF_3$, has attracted substantial interest as a model system for understanding phase transitions in $ABX_3$ systems like $MgSiO_3$. In this work, we have explored the high-pressure behavior of $NaMgF_3$ to ~160 GPa using laser-heated diamond cells coupled with *in situ* synchrotron x-ray diffraction. We show that the phase transition sequence in $NaMgF_3$ up to 162 GPa and 2500 K is: $NaMgF_3$ (perovskite) → $NaMgF_3$ (post-perovskite) → $NaMgF_3$ ($Sb_2S_3$-type) → NaF (B2-type) + $P2_1/c$-type $NaMg_2F_5$ → NaF (B2) + $MgF_2$ (cotunnite-type). Previous theoretical studies based on density functional theory have predicted a two-stage dissociation[1] of the post-perovskite (pPv) phase, first into $NaMg_2F_5$ + NaF at 29 GPa and then into NaF + $MgF_2$ at 71 GPa, while experiments suggested the pPv phase to be stable[2] at least up to 70 GPa and 2500 K or undergo a phase transition[3] at 37 GPa and 2000 K. Although, our results are in general agreement with the theoretical prediction, the dissociation reactions were found to occur at much higher pressures than the theoretically calculated value. Our work provides the first experimental evidence in any $MgSiO_3$ analogue compound for a high-pressure phase transition sequence involving a post-perovskite phase followed by two-stage dissociation. Notably, a similar sequence of transition is expected to occur in $MgSiO_3$ at ultra-high pressures where it has implications for the mineralogy and dynamics of large, rocky extra-solar planets.

**References**

[1] K. Umemoto and R.M. Wentzcovitch, Proceedings of the International Symposium "Nanoscience and Quantum Physics 2012" (NanoPHYS'12) **4**, 011002 (2015).

[2] B. Grocholski, S.-H. Shim, and V.B. Prakapenka, Geophys. Res. Lett. **37**, L14204 (2010).

[3] C.D. Martin, W.A. Crichton, H. Liu, V. Prakapenka, J. Chen, and J.B. Parise, Geophys. Res. Lett. **33**, L11305 (2006).