

Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

***Cmcm* post-perovskite: a new alumina polymorph**¹ JUN TSUCHIYA, TAKU TSUCHIYA, RENATA WENTZCOVITCH, University of Minnesota — Alumina, Al_2O_3 , is a model ceramic material with important applications in high pressure science, particularly as the ruby pressure scale. It is isoelectronic with MgSiO_3 , the major Earth forming mineral. Here we show by first principles that the newly found post-perovskite polymorph of MgSiO_3 , CaIrO_3 type structure with *Cmcm* symmetry, is also a stable high pressure phase of Al_2O_3 and should be stabilized in the pressure range in which the ruby scale has been calibrated. The sequence of polymorphs under pressure in these minerals is therefore analog: corundum/ilmenite \rightarrow *Pbnm*-perovskite for MgSiO_3 and $\text{Rh}_2\text{O}_3(\text{II})$ type for Al_2O_3 \rightarrow *Cmcm* post-perovskite. The reason for the greater stability of *Pbnm*-perovskite in MgSiO_3 versus $\text{Rh}_2\text{O}_3(\text{II})$ -type in Al_2O_3 is the difference in cation polyhedral types and volumes in the former, that favors for ABX_3 -type composition.

¹JSPS, NSF/EAR 013533 (COMPRES), 0230319, and NSF/ITR 0428774.

Jun Tsuchiya
University of Minnesota

Date submitted: 03 Dec 2004

Electronic form version 1.4