Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

d-Electrons' Occupancy and Crystal Structure in Transition Metal Sesquioxides[1] KOICHIRO UMEMOTO, Geology and Geophysics, University of Minnesota, RENATA WENTZCOVITCH, Chemical Engineering and Materials Science, University of Minnesota — We present a systematic density functional study of phase relations in transition metal sesquioxides: Y_2O_3, Rh_2O_3, and In_2O_3. Y_2O_3 and In_2O_3 undergo pressure-induced transitions accompanied by increase in cation coordination number from 6 to 7. However, in Rh_2O_3, such transition does not occur up to ~350 GPa. This cannot be explained simply arguments based on ionic radii ratios. Inspection of the electronic structure reveals that, in Rh_2O_3, the spatial distribution of the partially-occupied 4d states plays a very important role in the extraordinary stability of the Rh_2O_3(II)-type structure against others with higher coordination numbers. This study suggests that the complexity of phases in 3d/4d-transition-metal sesquioxides is not only due to ratio ionic radii but also by filling of the d states.

[1] Research supported by NSF grants ATM 0428774 (VLab) and EAR 0635990. Computations were performed at the Minnesota Supercomputing Institute.

Koichiro Umemoto
Geology and Geophysics, University of Minnesota

Date submitted: 17 Dec 2009

Electronic form version 1.4