Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Theory of magnesium silicates with bearing Fe and Al in the lower mantle and the Earth's D" layer[1] FEIWU ZHANG[2], ARTEM OGANOV[3], ETH Zurich — Although iron and aluminum incorporation into Earth's mantle minerals are expected to have important effects, little is known about Fe valence and spin state in such major phases as $MgSiO_3$ perovskite (*Pv*, main mineral of the lower mantle) and post-perovskite (*PPv*, main mineral of the Earth's D" layer). Here, we perform *ab initio* simulations, indicating that $Fe^{2+} \rightarrow Fe(metal) + Fe^{3+}$ in *Pv* & *PPv*. A new detailed microscopic picture of $MgSiO_3$ *Pv* & *PPv* is presented, including the complexity of Fe-Al incorporation, the spin transitions in Fe^{3+} and lack of such in Fe^{2+}, and the effects of Fe^{2+}, Fe^{3+}, Al^{3+} on the stability of *PPv*. These theory results explain and reconcile the recent diverse experimental results on the iron spin transition in $MgSiO_3$ and provide basis for future geodynamical and petrological studies of the mantle and the D" layer.

[1]Acknowledge access to supercomputers at CSCS (Manno) and the HP Superdome of ETH Zurich. Funding by ETH Zurich
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Date submitted: 25 Nov 2005 Electronic form version 1.4