

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

The Phase Diagram of Portlandite, Ca(OH)_2 at Pressures up to 40 GPa BORIS KIEFER, MEGAN LOCKWOOD, Department of Physics; New Mexico State University — Hydroxides have attracted significant scientific interest over the past decades. They have been used as analogues to further our understanding of hydrogen bonding in complex materials. Several experimental observations suggest that portlandite undergoes reversible solid state amorphization at high pressures but the cause for this transition and its appearance in portlandite remains unknown. We performed static (0 K) first-principle calculations based on the GGA within the framework of Density-Functional-Theory in order to explore the phase diagram of portlandite for pressures up to 40 GPa. All structures were fully relaxed to determine the ground state of portlandite. We find that a split-site model for the hydrogen array is energetically preferred consistent with neutron diffraction experiments. At a pressure of ~ 4.5 GPa we observe a phase transition from trigonal to monoclinic symmetry in agreement with previous studies. At all higher pressures we find that the monoclinic structure is the ground state of portlandite. However, we identified several energetically comparable structures. This indicates that the potential energy surface of portlandite has a surprisingly complex structure. The interplay of these structures suggest that the solid state amorphization is driven by non-hydrostatic stress and allows to rationalize experimentally observed differences between portlandite powders and single-crystals.

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Date submitted: 27 Nov 2007

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