

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

New high-pressure phases of calcium and their finite-temperature phase boundaries¹ AMANUEL TEWELDEBERHAN, Dalhousie University, STANIMIR BONEV, Dalhousie University — The phase diagram of Ca has been studied using first-principles density functional theory. The simple cubic structure hitherto believed to exist between 32 and 109 GPa is found to be mechanically and thermodynamically unstable. Instead we propose two new solid phases with orthorhombic *Cmcm* and *Pnma* structures and determine their finite-temperature phase boundaries. We also predict liquid transitions in molten Ca under compression, which together with the new solid phases provide a consistent description of the Ca phase diagram. The implications of our findings and extensions of the work to other alkali and alkaline-earth metals will be discussed.

¹Work supported by NSERC and ACEnet.

Amanuel Teweldeberhan
Dalhousie University

Date submitted: 21 Nov 2008

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