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A high PT scale based on density functional calculations of MgO<sup>1</sup> Z. WU, R.M. WENTZCOVITCH, Department of Chemical Engineering and Materials Science and Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN 55455, USA, B. LI, Mineral Physics Institute, Stony Brook University, Stony Brook, NY 11794, USA, K. UMEMOTO, Department of Chemical Engineering and Materials Science and Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, MN 55455, USA — In situ crystallography based on diamond anvil cells have recently been extended to the multi-Mbar regime. Temperatures in these experiments have crossed the 2,000 K mark. Yet, current high PT standards of calibration produce too large uncertainties to the point of inhibiting clear conclusions regarding the importance of certain phenomena for planetary processes at these high PTs, e.g., the post-perovskite transition in Earths mantle. We propose a calibration based on thermal equations of state (EoS) of MgO obtained from LDA quasiharmonic (QHA) calculations. These EoSs agree very well with several calibrations at relatively low PTs. This gives further support to our predictions made within the range of validity of the QHA.

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