

Abstract Submitted
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Consistent first-principles pressure scales for diffraction experiments under extreme conditions ALBERTO OTERO-DE-LA-ROZA, School of Natural Sciences, University of California, Merced, 5200 North Lake Road, Merced, California 95343, USA, VICTOR LUÑA CABAL, Departamento de Química Física y Analítica, Facultad de Química, Universidad de Oviedo, ES-33006 Oviedo, Spain — Diamond anvil cell (DAC) diffraction experiments are fundamental in geophysics and materials science to explore the behavior of solids under very high pressures and temperatures. A factor limiting the accuracy of DAC experiments is the lack of an accurate pressure scale for the calibration materials that extends to the ever-increasing pressure and temperature limits of the technique. In this communication, we address this problem by applying a newly developed technique that allows the calculation of accurate thermodynamic properties from first-principles calculations [Phys. Rev. B 84 (2011) 024109, 84 (2011) 184103]. Three elements are key in this method: i) the quasiharmonic approximation (QHA) and the static energies and phonon frequencies obtained from an electronic structure calculation ii) the appropriate representation of the equation of state by using averages of strain polynomials and iii) the correction of the systematic errors caused by the exchange-correlation functional approximation. As a result, we propose accurate equations of state for typical pressure calibrants that can be used in the whole experimental range of pressures and temperatures. The internal consistency and the agreement with the ruby scale based on experimental data is examined.

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