

Abstract Submitted
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High-pressure phases of calcium¹ AMANUEL TEWELDEBERHAN, JONATHAN DOBOIS, Lawrence Livermore National Laboratory, STANIMIR BONEV, Lawrence Livermore National Laboratory and Dalhousie University — The high-pressure phases of calcium have been investigated using a combination of density functional theory and diffusion quantum Monte Carlo calculations. Finite-temperature Gibbs free energies of several competing structures are computed at pressures near 50 GPa. The discrepancy between theory and experiment both at low and room temperature is resolved with input from diffusion quantum Monte Carlo. Furthermore, diffusion quantum Monte Carlo calculations are performed on 0 K crystalline structures up to 150 GPa. The resulting structures differ from those obtained with density functional theory.

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