

Abstract Submitted  
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**Thermodynamic properties of solids and liquids at extreme conditions**<sup>1</sup> AMANUEL TEWELDEBERHAN, Lawrence Livermore National Lab, STANIMIR BONEV, Lawrence Livermore National Lab and Dalhousie University — A recent work on high pressure phases of calcium using a combination of density functional theory and diffusion quantum Monte Carlo methods will be presented. Various approaches have been used to compute the entropies and free energies of different structures of calcium exhibiting strong anharmonicity to account for their thermodynamic stability at high pressure. We will also discuss efficient methods for computing liquid free energies and their application to predict mixing and de-mixing behavior in low-Z liquid mixtures at high pressure and temperature.

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