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Highly Accurate Calculations of the Phase Diagram of Cold Lithium LUKE SHULENBURGER[1], ANDREW BACZEWSKI, Sandia National Laboratories — The phase diagram of lithium is particularly complicated, exhibiting many different solid phases under the modest application of pressure. Experimental efforts to identify these phases using diamond anvil cells have been complemented by ab initio theory, primarily using density functional theory (DFT). Due to the multiplicity of crystal structures whose enthalpy is nearly degenerate and the uncertainty introduced by density functional approximations, we apply the highly accurate many-body diffusion Monte Carlo (DMC) method to the study of the solid phases at low temperature. These calculations span many different phases, including several with low symmetry, demonstrating the viability of DMC as a method for calculating phase diagrams for complex solids. Our results can be used as a benchmark to test the accuracy of various density functionals. This can strengthen confidence in DFT based predictions of more complex phenomena such as the anomalous melting behavior predicted for lithium at high pressures.

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