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Quantum Monte Carlo applied to Solids under Pressure LUKE SHULENBURGER, T.R. MATTSSON, Sandia National Laboratories — Diffusion quantum Monte Carlo (DMC) has been applied to solids under pressure in several different contexts a high degree of success.[1] All of these calculations must address three errors present in DMC calculations of solids: the fixed node approximation, the pseudopotential approximation and the finite size approximation. Due to the varying approximations to address these errors, these calculations suffer from an uncertainty that is almost comparable to that introduced by the choice of functional in density functional theory (DFT). In this presentation, we present lattice constants and bulk moduli of more than fifteen solids under compression performed with a consistent approach to these three approximations. These results help establish the general accuracy that may be expected from DMC calculations of solids under pressure and also provide a reference from which improvements to DMC methods may be judged.

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[1]J. Kolorenc and L. Mitas. Rep. Prog. Phys. 74 026502 (2011)

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