Tin phase transition in terapascal pressure range described accurately with Quantum Monte Carlo. ROMAN NAZAROV, RANDOLPH HOOD, MIGUEL MORALES, Lawrence Livermore Natl Lab — The accurate prediction of phase transitions is one of the most important research areas in modern materials science. The main workhorse for such calculations, Density functional theory (DFT), employs different forms of approximate exchange-correlation functionals which may lead to overstabilization of one phase compared to another, therefore, predict incorrectly phase transition pressures. A recent example of such deficiency has been demonstrated in Sn: no bcc to hcp phase transition has been observed in Sn when dynamically compressed to 1.2 TPa while DFT predicts a transition to occur at 0.16-0.2 TPa [1]. To overcome the limitations of DFT, we have employed diffusion quantum Monte Carlo (DMC) method which treats the many body electron problem directly. In order to get highly accurate results we systematically assess the effect of controllable approximations of DMC such as fixed node approximation, finite-size effects and the use of pseudopotentials. Based on metrologically accurate DMC equation of states we construct the pressure-temperature phase diagram and demonstrate its good agreement with experiment in contrast to DFT calculations. [1] A. Lazicki et al., X-Ray Diffraction of Solid Tin to 1.2 TPa. Phys. Rev. Lett. 115, 075502 (2015).

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