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Quantum Monte Carlo calculations of bulk Li KEVIN RASCH, LUBOS MITAS, North Carolina State University — Using all-electron fixed-node quantum Monte Carlo methods we calculate equations of states for ambient and high pressure phases of Li using the structural data from experimental observations up to high pressures.[1] We compare the suitability of orbital sets from several Density Functional Theory functionals for use in many-body trial Slater-Jastrow wavefunctions. We reduce finite-size errors by utilizing twist-averaging[2] and by structure factor correction for several sizes of simulation cell.[3]

[1]M. Hanfland, K. Syassen, N. E. Christensen, and D. L. Novikov, Nature 408, 174–178 (2000).
[2]C. Lin, F. H. Zhong, and D. M. Ceperley, Phys. Rev. E 64, 016702 (2001).
[3]S. Chiesa, D. M. Ceperley, R. M. Martin, and M. Holzmann, Phys. Rev. Lett. 97, 076404 (2006).

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