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Cold melting of Li under pressure: Perspectives from first-principles molecular dynamics simulations[1] WEIYI XIA, WEIWEI GAO, Department of Physics, University at Buffalo, SUNY, Buffalo, NY 14260, USA, XIANG GAO, Beijing Computational Science Research Center, Beijing, China, 100084, PEIHONG ZHANG, Department of Physics, University at Buffalo, SUNY, Buffalo, NY 14260, USA — Despite much work (experiment and theory), the pressure-dependent melting temperature of Li is still under debate. In particular, there is still controversy and significant uncertainty in determining the melting temperature of Li at pressures around 50 GPa. An earlier report [1] suggests that Li melts at as low as 190 K between 40 and 64 GPa. Such a low melting temperature is not likely unless quantum effects of lattice vibration play a significant role. Later experiment [2], on the other hand, reports that Li melts above 300 K under pressured up to 64 GPa and does not seem to support the view that lattice quantum effects to play any important role. In this talk, we will present results from large-scale (large systems and long simulation times) first-principles molecular dynamics simulations and phonon free energy calculations, aiming at resolving some of the issues. [1] C.L. Guillaume et al, Nature Phys. 7, 211 (2011). [2] A. M. J. Schaeffer et al, Phys. Rev. Lett. 109, 185702 (2012). [3] F.A. Gorelli et al, Phys. Rev. Lett. 108, 055501 (2012).

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