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On the role of quantum ion dynamics for the anomalous melting of lithium[1] SABRI ELATRESH, Department of Physics, Dalhousie University, Halifax, NS, B3H 3J5, Canada, STANIMIR BONEV, Lawrence Livermore National Laboratory, Livermore, California 94550 — Lithium has attracted a lot of interest in relation to a number of counterintuitive electronic and structural changes that it exhibits under pressure. One of the most remarkable properties of dense lithium is its anomalous melting. This behavior was first predicted theoretically based on first-principles molecular dynamics (FPMD) simulations, which treated the ions classically [1]. The lowest melting temperature was determined to be about 275 K at 65 GPa. Recent experiments measured a melting temperature about 100 K lower at the same pressure. In this talk, we will present FPMD calculations of solid and liquid lithium free energies up to 100 GPa that take into account ion quantum dynamics. We examine the significance of the quantum effects for the finite-temperature phase boundaries of lithium and, in particular, its melting curve.

[1] I. Tamblyn, J-Y. Raty, and S. A. Bonev, Phys. Rev. Lett. 101, 075703 (2008).
[2] E. Gregoryanz et al, Nature, in press.

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