

Abstract Submitted
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Clustering in dense molten lithium¹ ISAAC TAMBLYN, Dalhousie University, JEAN-YVES RATY, University of Liege, STANIMIR A. BONEV, Dalhousie University — Molten lithium is investigated from zero to over nine-fold compression using first principles theory. Over this pressure range, we observe several electronic and structural transitions. The changes that lithium undergoes with increasing pressure are initially analogous to those predicted for liquid sodium [1]. However, upon further compression, effects due to increased core overlap lead to a new liquid phase composed of weakly bound lithium clusters. The properties of the proposed new liquid phases, the melting curve of lithium, and the implications of our findings for the stability of low-symmetry lithium solids will be discussed. [1] J.-Y. Raty, E.R. Schwegler, S.A. Bonev, *Nature*, 449, 448-451 (2007)

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