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Computer Simulation Evidence for a Liquid-Liquid Phase Transition in Gallium: Bulk and Nanodroplets[1] ALEX ANTONELLI, DIEGO JARA, MATEUS MICHELON, MAURICE DE KONING, Universidade Estadual de Campinas — Over the last decade, there has been an increasing interest in the first-order liquid-liquid phase transition (LLPT) between liquids of the same chemical composition. While LLPT has been speculated to occur in several liquids that exhibit anomalies in their thermodynamic properties, so far in only two cases it has been experimentally verified. This lack of evidence stems from difficult experimental conditions, since in many cases the LLPT is expected to occur in the metastable supercooled regime. Gallium is a very promising substance for the study of LLPT, since it has low melting point (303 K), displays anomalous behavior, and can be kept liquid about 100 K below its melting temperature. In this work, we report on molecular dynamics simulations of liquid Ga that provide theoretical evidence of a LLPT from a high density to a low density liquid in bulk [1] and nanodroplets. Our results indicate a reduction in the temperature and latent heat of the LLPT as the size of the system decreases. [1] D. A. C. Jara, M. F. MIchelon, A. Antonelli, and M. de Koning, Journal of Chemical Physics **130**, 221101 (2009).

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