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Entropic changes in liquid gallium clusters: understanding the anomalous melting temperatures NICOLA GASTON, MacDiarmid Institute for Advanced Materials and Nanotechnology, KRISTA STEENBERGEN, Massey University — Melting in finite-sized materials differs in two ways from the solid-liquid phase transition in bulk systems. First, there is an inherent scaling of the melting temperature below that of the bulk, known as melting point depression. Secondly, at small sizes, changes in melting temperature become non-monotonic, and show a size-dependence that is sensitive to the structure of the particle. Melting temperatures that exceed those of the bulk material have been shown to occur in vacuum, but have still never been ascribed a convincing physical explanation. Here we find answers in the structure of the aggregate liquid phase in small gallium clusters, based on molecular dynamics simulations that reproduce the greater-than-bulk melting behavior observed in experiments, and demonstrate the critical role of a lowered entropy in destabilising the liquid state.

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