Abstract Submitted
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Greater-than-bulk melting temperatures explained: Gallium melts Gangnam style NICOLA GASTON, Victoria University of Wellington, KRISTA STEENBERGEN, Freie Universitaet Berlin — The experimental discovery of superheating in gallium clusters [1] contradicted the clear and well-demonstrated paradigm that the melting temperature of a particle should decrease with its size. However the extremely sensitive dependence of melting temperature on size also goes to the heart of cluster science, and the interplay between the effects of electronic and geometric structure. We have performed extensive first-principles molecular dynamics calculations, incorporating parallel tempering for an efficient exploration of configurational phase space. This is necessary, due to the complicated energy landscape of gallium. In the nanoparticles, melting is preceded by a transitions between phases. A structural feature, referred to here as the Gangnam motif, is found to increase with the latent heat and appears throughout the observed phase changes of this curious metal. We will present our detailed analysis of the solid-state isomers, performed using extensive statistical sampling of the trajectory data for the assignment of cluster structures to known phases of gallium. Finally, we explain the greater-than-bulk melting through analysis of the factors that stabilise the liquid structures.

[1] G. A. Breaux, et al, Phys. Rev. Lett. 91, 215508 (2003)

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