

Abstract Submitted
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Monte Carlo simulations of Phase Changes in Lennard-Jones nanoclusters. SILVINA GATICA¹, Department of Physics and Astronomy, Howard University, XIAO DONG, ESTELA BLAISTEN-BAROJAS, School of Computational Sciences, George Mason University — Monte Carlo simulations of Lennard-Jones clusters of less than 100 atoms are performed to explore the possible phase changes. The simulation is made at constant pressure and temperature. In the Monte Carlo the volume of the cluster is evaluated during the calculation in terms of the mean quadratic radius, and the reduced temperature is kept below 0.4 to avoid the evaporation of the cluster. We obtain a PV diagram and calculate the energy per particle, the radial distribution function, the coordination number and displacement function, to look for signatures of the presence of a solid-liquid-like phase change. The equilibrium structure and number of layers in the cluster at each pressure and temperature are also computed. We compare our findings with predictions of other authors.

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