Abstract Submitted
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Energetics and equation of state of passivated nanocluster assemblies[1] W.D. LUEDTKE, UZI LANDMAN, School of Physics, Georgia Institute of Technology — Molecular dynamics simulations are used to explore several principal issues pertaining to the energetics of formation of superlattices made through the assembly of passivated nanoclusters and the interactions that underlie the cohesion of such superlattices [1]. The entropic contribution to the formation free energy of the superlattice assembly is found to be large and of similar magnitude as the potential energy component of the free energy. The major contribution to the cohesive potential energy of the superlattice is shown to originate from van der Waals interactions between molecules that passivate neighboring nanoclusters. Additionally, we have found that a passivated nanocluster assembly can undergo pressure induced structural transformations and we discuss the equation of state of such superlattice assemblies. [1] U. Landman and W. D. Luedtke, Faraday Discussions 125, 1 (2004).

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