Pressure Induced the Phase Transition in Nano-cluster and Carbon Nano-tubes

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Studies on the phase transition of the nano-cluster and nano-tubes recently become very interesting. In this talk I present a new method for constant-pressure molecular dynamics simulation which is parameter free. This method is especially appropriate for finite systems in which a periodic boundary condition does not apply. I will also show the results on the pressure induced phase transition in carbon nanotubes and nano-clusters, from which one can also easily obtain the equations of states for a finite system under external pressure.