Pressure-driven phase transitions in nanoparticles

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There is currently much interest in the controlled synthesis of nanocrystals, driven both by the continuing minaturisation of electronic components, and by the possibility that exploiting size effects may give control over the physical properties of such materials. A Caesium Chloride potential has previously been developed to study the B1 to B2 pressure-driven phase transition in the bulk system, using constant pressure molecular dynamics simualtion. This same potential has been used to model simple nanocrystals which have been embedded in a binary Lennard-Jones fluid and then compressed in order to study the finite size effects on this phase transition.