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Molecular dynamics studies of some carbon nanotubes chiral structures

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Abstract content
 (Max 300 words)
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Structural and equilibrium properties of armchair (cnt(12,12)) and two chiral (cnt(10,12) and cnt(12,10)) carbon nanotubes are studied using classical molecular dynamics. The formulation uses the Tersoff potential under the NVT ensemble to study these properties. Structural properties are studied using the radial distribution and structure factor functions. The equilibrium properties are studied using the total energy against lattice parameter variation. Similarities and differences in cnt(12,12), cnt(10,12), and cnt(12,10) symmetries are discussed.

Apply to be considered for a student award (Yes / No)?

No

Level for award (Hons, MSc, PhD)?

none

Would you like to submit a short paper for the Conference Proceedings (Yes / No)?

Yes

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