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Computational study of some Carbon modification

Thursday, 14 July 2011 17:00 (2 hours)

<p>Classical molecular dynamics simulations were used to study the modification of some carbon forms. The type of carbons that were used is diamond and nanocarbon. Carbon is unique among other elements in its ability to form strong chemical bonds with a variety of coordination numbers. The simulations predict that the behaviour of diamond and nanocarbon are similar although the nanotube has low minimum energy compared to the bulk diamond. The radial distribution functions of the two forms differ by half a magnitude.

Level (Hons, MSc,
   PhD, other)?

MSc

Consider for a student
   award (Yes / No)?

No

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

yes

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