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Thermal expansion, elastic modulus and phase transition of carbyne: A stochastic model of chemical bonds distribution

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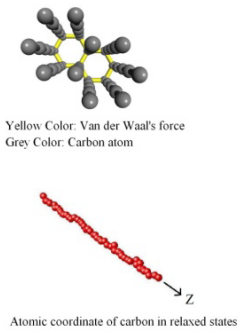
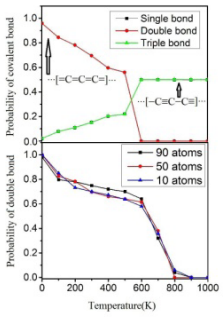
A plenty of theoretical studies have been conducted by DFT to predict the physical properties of carbon chain. In the present work we develop a powerful Monte Carlo algorithm of the carbon chains ordered into 3D hexagonal array. Our group develops a new routine to probe the phase transition between the alpha and beta carbyne based on the chemical bond and atomic distributions. Our model confirms that the cumulene phase is more energetic preferable at low temperatures but the carbon chain prefers to switch into polyvine phase at high temperatures. The bond softening temperature is observed at 480 K. The larger bond softening temperature is observed in the presence of interstitial doping but it does not show length-dependence. The elastic modulus of the carbon chains is 1.7 TPa at 5 K and the thermal expansion is +70 μ K-1 at 300 K via monitoring the resultant atomic vibrations and bond distributions. Thermal fluctuation in terms of heat capacity as a function of temperatures shows that the melting point is around 3800 K. The carbon atoms along the carbon nanowire arranged in relaxed state is displayed at the end.





Biography

C H Wong has his expertise in Monte Carlo simulation and *ab-initio* calculation in material science. He has passion in searching for 300 K superconductors. He has joined in an experimental physics group and was trained to conduct AC calorimetry in the resolution better than 5 decimal places during his Doctoral degree in Hong Kong. He made contributions in capturing tiny superconducting signals in nanostructured materials and also discovered more fundamental physics of superconductors based on the ultra-weak heat capacity anomaly. After he graduated in 2015, he explores in theoretical condensed matter physics as a Postdoctoral Researcher in Russia, in order to design high temperature superconductors from theoretically point of view. He has constructed a stochastic model for carbon nanowire carrying extremely large Debye frequency and proposes the algorithm towards stabilized carbon nanowires array.

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