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Influence of pressure and defects on CNT interlinking

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Carbon nanotubes (CNT's) have a variety of different uses, in nanoscience and nanotechnology, such as energy storage, device modelling, automotive parts, thin-film electronics etc. Due to the large range of applications understanding the characteristics and typical behaviour of these materials becomes important. In realistic systems, CNT's will contain defects such as adatoms and vacancies and be exposed to pressure changes.

It has been shown both theoretically and experimentally that when sufficient pressure is applied to an isolated, pristine CNT it can result in a structural deformation and can provide a means to change sp_2 to sp_3 bonds which at times leads to interlinking/bonding between CNTs in the material. [1] The applied pressure resulted in stronger harder materials with pressure tuneable band gaps. [2]

Experimentally, interlinking between tubes has been observed when defects are introduced into systems. Similarly to pressure, the cross-linking effect caused can be used to modify the material properties. [3, 4, 5]

The modification of the different electronic, optical, and mechanical changes accompanying these behaviours highlight the impact of understanding the effect of pressure and defects on CNT's. In this work we theoretically study the effects of pressure combined with different defects for various sizes and chiralities of CNT. We further use this to predict when the bond type will change and when interlinking is most likely to occur in a CNT system.

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