Contribution ID: **96** Type: **Oral Presentation**

Structural determination and electronic properties of one-dimensional Te crystals encapsulated inside carbon nanotubes

Wednesday, 13 July 2016 11:55 (20 minutes)

Abstract content
   (Max 300 words)
Formatting &
Special chars

We use the ab initio random structure searching (AIRSS) method to determine the geometries of one-dimensional (1D) nanowires formed by encapsulating Te atoms inside single-walled carbon nanotubes (SWCNT). Particular attention is given to narrow SWCNTs (NSWCNTs) with diameters between 5 and 11 Aring;, since chemical interactions between such NSWCNTs and the encapsulated Te atoms are, in principle, more likely to occur than in SWCNTs with larger diameters. We show that there is a clear preference for the confined Te atoms to form 1D nanowires with helical symmetry. Also, despite the small diameters of the NSWCNTs studied, we show that chemical interactions between the encapsulated nanowires and the NSWCNTs do not play a crucial role in determining the geometries of the most energetically favourable structures. The calculated structural parameters of the encapsulated nanowires are in excellent agreement with the structures synthesised in our experiments. A comparison between our theoretically predicted and experimentally measured electronic and spectroscopic properties shows that our combined theoretical-experimental approach allows for a very precise characterisation of such systems.

Primary author: Dr MEDEIROS, Paulo V C (Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, U.K.)

Co-authors: Dr MORRIS, Andrew J. (Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, U.K.); Dr QUIGLEY, David (Department of Physics, University of Warwick, Coventry CV4 7AL, U.K. and Centre for Scientific Computing, University of Warwick, Coventry CV4 7AL, U.K.); Mr WYNN, Jamie M. (Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, U.K.); Dr SLOAN, Jeremy (Department of Physics, University of Warwick, Coventry CV4 7AL, U.K.); Dr MARKS, Samuel (Department of Physics, University of Warwick, Coventry CV4 7AL, U.K.)

Presenter: Dr MEDEIROS, Paulo V C (Theory of Condensed Matter Group, Cavendish Laboratory, University of Cambridge, J. J. Thomson Avenue, Cambridge CB3 0HE, U.K.)

Session Classification: Parallel Track B