Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Structure of carbon-nanotube-encapsulated nanowires from first principles calculations JAMIE WYNN, PAULO MEDEIROS, University of Cambridge, JEREMY SLOAN, DAVID QUIGLEY, University of Warwick, ANDREW MORRIS, University of Cambridge — The quasi-1D structures formed by the insertion of materials into carbon nanotubes can differ dramatically from bulk phases in their structures and properties. Many of these encapsulated nanowire (ENW) structures have considerable technological potential, in areas such as phase-change memory and gas sensing. However, the structures of ENWs can also bear little resemblance to their bulk forms. We have therefore adapted the *ab initio* random structure search (AIRSS) method for the prediction of the structures of nanowires encapsulated inside carbon nanotubes. The AIRSS method has previously proven itself as a powerful and effective tool in the prediction of both bulk materials [1] and defect complexes [2]. Using AIRSS, we have predicted the structure formed by germanium telluride ENWs as a function of the radius of the encapsulating nanotube. We use simulated TEM imagery to show that our results are consistent with experimental evidence [3].

[1] M Mayo, KJ Griffith, CJ Pickard, AJ Morris, Chemistry of Materials 28 (7), 2011-2021
[2] AJ Morris, CJ Pickard, RJ Needs, Physical Review B 78 (18), 184102
[3] C Giusca et al., Nano Lett. 13 (9), 4020

Jamie Wynn
University of Cambridge

Date submitted: 15 Nov 2016 Electronic form version 1.4