University of BRISTOL

Functionalisation of chevron type graphene nanoribbons

Mat Tolladay[1], Neil L. Allan[2], and Fabrizio Scarpa[1]

[1]Advanced Composites Centre for Innovation and Science (ACCIS), University of Bristol, Queen's Building, University Walk, Bristol, BS8 1TR, United Kingdom.
[2]School of Chemistry, University of Bristol, Cantock's Close, Bristol, BS8 1TS, United Kingdom.

Abstract

Nanocomposite materials usually consist of two materials: reinforcing particles and a polymer matrix. To ensure load transfer between the nanoparticles and the polymer a bond must be formed between them. The stronger the bond between the constituents the better the load transfer and the stronger the material. One potential reinforcement is graphene nanoribbons, thin strips of graphene, which could potentially be connected to polymer chains via covalent bonds. Recently a variation of these nanoribbons, chevron type nanoribbons, have been produced using on surface production from molecular precursors and cyclodehydrogenation. These zig-zag shaped ribbons have a higher edge to length ratio than straight nanoribbons and may therefore also provide a higher density of covalent bonds per unit length. This work explores functionalisation of nanoribbons with the aim to find the most probable sites for functionalisation. Density functional theory is used to predict the structure of graphene nanoribbons with hydrogen adatoms at different positions on the lattice. Energetic, structural and mechanical consequences of the presence of the adatoms are examined in detail.

Acknowledgements

This work was supported by the Engineering and Physical Sciences Research Council through the EPSRC Centre for Doctoral Training in Advanced Composites for Innovation and Science [grant number EP/L016028/1]