Y Hancock, J Nanomed Nanotechnol 2016, 7:4 (Suppl)
http://dx.doi.org/10.4172/2157-7439.C1.040

9th Nano Congress for Next Generation

August 01-02, 2016 Manchester, UK

Nanographene device design

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Advances in the production of nanographene using top-down fabrication, e.g., e-beam lithography, or by bottom-up, surface-assisted chemical synthesis have provided much impetus to directly link theory and experiment. The benefits are two-fold. On the theoretical-side this allows the development of more accurate models by direct comparison of simulation with experimental measurement. Such comparisons are vital for understanding the 'missing' physics in the theoretical modelling of nanographene. On the experimental side, the creation of accurate, theoretical design tools can greatly reduce experimental trial and error, thus opening the potential for efficient quantum engineering and device discovery. Theoretically-informed experiments can also circumvent time-consuming and often expensive procedures in determining specific features (size, functionalisation, patterning, etc.) for targeted applications and new intellectual property. To meet these aims, we have developed a computationally and physically transparent minimal model for nanographene coupled to a 'graphene user interface' or GRUI. The minimal model is computational efficient against density functional theory, and can reach large unit cell sizes for realistic modelling. The GRUI can also be directly interfaced with experiment and employed for rapid predictive simulation in nanographene device design. We will demonstrate the accuracy of the method and portray example results (e.g., spin transport) pertaining to our work on patterned and defected graphene nanoribbon devices (top-down), and for chemically-synthesised nanographene (bottom-up) determined via directed, kinetic self-assembly simulation.

Biography

Y Hancock obtained her PhD in 2003 at Monash University in Theoretical Quantum Physics and Engineering of Nanoscale Technologies. After completing a Post-doc at Monash, she moved to Aalto University (2006-2009) where she became Research Manager of a large-scale collaboration with Nokia supervising projects on next-generation mobile technologies. In 2009, she was appointed as Lecturer at the University of York where she works with her group on graphene studies and in the field of biomedical research.

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