

Multi-functional Graphene/Carbon Nanotube Nanocomposites

Prof. Michael A. McCarthy^a, Dr. Chunyu Li^a, Dr. Daniel M. Mulvihill^a, Prof. William A. Curtin^b

^aDept. of Mechanical, Aeronautical, and Biomedical Engineering, University of Limerick

^bInstitute of Mechanical Engineering, École Polytechnique Fédérale de Lausanne, Switzerland

Contact Email: michael.mccarthy@ul.ie

Abstract

This proposal addresses the Grand Challenge of realising the enormous potential for using graphene and carbon nanotubes (CNTs) in polymer matrices to achieve multi-functional Graphene/CNT nanocomposites. Multifunctional materials are capable of meeting multiple demands, such as structural, electrical, thermal, and energy storage for example. Many technical challenges must be overcome before such materials reach a point where they are a viable commercial alternative to traditional micron-sized carbon-fibre composites, and computational science can play a major role in accelerating this development process. Funding has been secured for two outstanding postdoctoral fellows to work on this topic, and this proposal seeks to secure the computational resources needed for their work. A Marie Curie IIF-funded fellow will model mechanical, thermal, and electrical properties of multifunctional thermoset nanocomposites where the reinforcement is a novel graphene-CNT hybrid mix. Large-scale molecular dynamics simulations, combined with custom routines for modelling of in-situ curing and the formation of percolation networks will be used to determine the compositions and arrangements of nanofillers which give optimum mechanical, thermal and electrical properties. An Irish Research Council fellow will focus on a narrower but absolutely critical aspect of the problem; namely, the problem of optimising load transfer to the individual graphene sheets in graphene nanocomposites. While the mechanical properties of single-layer pure graphene are extraordinary, the full strength potential of graphene as a reinforcement in composite materials remains unrealised due to poor load transfer. This part of the work will investigate how functionalisation of graphene (the addition of functional groups to the basic graphene sheet) can improve load transfer between the graphene and the polymer matrix by enhanced interfacial bonding. Various methods of achieving improved interlayer bonding between the graphene sheets themselves in few-layer graphene nanoplatelets (GNPs) will also be studied. A combination of molecular dynamics and quantum mechanics simulations will be used to examine in detail the effects of the different kinds of functionalisation, as well as to optimise the inter-layer covalent bonding. The quality of the science and its potential impact is high, and the proposed work is extremely computationally intensive; therefore, Class A resources are required.