## PhD Studentship in Multiscale Modelling for Optimum Processing of Polymer-Graphene Nanocomposites

**Project Overview:** Polymers filled with multifunctional nanoparticles such as graphene are promising material candidates for producing multifunctional components/devices for use in sectors such as energy storage, flexible electronics, electromagnetic shielding. One of the main challenges in achieving optimum multifunctional properties is to obtain optimum dispersion and distribution of nanoparticles in the polymer. Melt state and quasi-solid state manufacturing processes offer means for controlling nanocomposite morphology, and hence of their end-use properties. However, those processes require a careful selection of optimum processing conditions to fully control the morphology, and thus end-use properties.

The ultimate objective of this project is to develop an advanced 3D nonlinear multiscale (molecular-continuum) computational model for the prediction and optimisation of the melt and quasi-solid state processing of polymer nanocomposites. The model development will address reconstruction of 3D nanocomposite morphologies using a Monte Carlo-like approach, and incorporation of the effects of nanoparticle functionalization by means of continuum constitutive laws predicted from simulations at the molecular level.

The successful candidate will be based in the International Institute for Nanocomposites Manufacturing (IINM), where the model will be experimentally-validated.

Awards available: 1 award available.

Funding Details: Fees and maintenance at RCUK Level

**Length of Award:** 3.5 years (PhD)

**Eligibility:** Due to funding restrictions, the position is only available for well-qualified UK or EU students. Other motivated students are encouraged to apply but will need to secure their own funding. Candidates should hold a 1<sup>st</sup> or 2.1 degree in any science or engineering discipline which had a significant materials/engineering simulation content.

**Application Details**: This project is available to start as soon as possible. Please contact Dr Łukasz Figiel by email (<a href="mailto:l.w.figiel@warwick.ac.uk">l.w.figiel@warwick.ac.uk</a>) with informal enquires about this project. Please apply directly via PG Admissions and note the reference number. Click here for the application form: <a href="mailto:http://go.warwick.ac.uk/pgapply">http://go.warwick.ac.uk/pgapply</a>