MECHANIC: Modelling Charge and Heat Transport in 2D-materIals based Composites

Main area: BSR06_Modelling charge and heat transport in GRM - based composites
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Abstract

Polymer-composites based on Graphene and related materials (GRM), such as thermoplastics and conductive flexible materials, hold promise for several key European industrial areas including aerospace and automotive industries where they find use in coating of batteries and cables, de-icing etc. The composites of most interest comprise structurally complex membranes of Graphene Oxide (GO) and reduced Graphene Oxide (rGO). These are disordered on multiple length scales and incorporate local geometrical defects, as well as a large amount of functional groups on GO/rGO. However, partners in the Flagship Core consortium (CNR, WP14) and companies (AVANZARE, WP15) lack knowledge to interlink their measurements of electrical and thermal conductivities with the complexity of the material morphology. For this reason, the MECHANIC-project targets modelling of charge and heat transport in highly disordered (realistic) GO/rGO thin films, as they appear in composites.We conceive a multi-scale approach spanning from the nano- to the macro-scale, deliberately including any structural/chemical complexity of laboratory samples. We will model charge and heat transport using semi-empirical methods, focussing on trends which can only be provided by large-enough computational samples. We will ensure accuracy by using ab-initio, in particular DFT, to extract local quantities and generate input data for the training of interatomic model potentials. Experimental input will be used both for sample-construction and model validation. Hence, the MECHANIC project will move beyond the state-of-the-art by considering transport in large and realistic disordered systems. This will provide meaningful and trustworthy insights on the transport physics and serve as design guides for GRM-composites in the Flagship. The ultimate goal is to accurately predict and control transport in various GO and rGO samples and GO/rGO interfaces with a view to improve efficiency and functionally enrich GO-based composite materials.MECHANIC brings together expertise from modelling on different scales, from the ab-initio level to the continuum scale and is characterized by a high level of interaction between nodes. CHALMERS will coordinate and provide interatomic force models together with TB-potentials from UCL who has expertise in first-principles modelling of carbon-based nanostructures. The potentials will be used for mesoscale heat and charge transport calculations by ICN2 (tight binding simulations of defected GRM structures), IZ-TECH (influence of nano-structuring and disorder on heat and charge transport) and UNICA (thermal transport calculations in 2D materials using MD). Prof. Palermo (CNR, WP14) and Dr. Gomez (AVANZARE, WP15) joins the consortium as associated members to ensure a strong connection and relevance of the work to experimental activities within the Flagship. Importantly we will continuously compare our results and structures with experimental data for model validation.

Consortium

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