Chemical functionalization of graphene surface as filler for rubber compounds: modeling of supramolecular interactions

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Over the last few years, the surface modification of fillers for high-level technological applications such as polymer composites for tyre industry, conductive inks and coatings has seen a considerable increase in interest since it can increase mechanical, electrical, and thermal properties of the final material. Nano-sized carbon allotropes such as graphene and carbon nanotubes are a suitable class of compounds for these purposes: high thermal and electrical conductivity along with considerable mechanical reinforcement are the main improvements that these fillers bring to the composite and their elevated surface area allows to reduce the filler volume ratio compared to more common alternatives. An efficient and reliable method to modify the surface of these nano-fillers is the so-called pyrrole methodology, [1] a mild procedure that involves bio-sourced reagents to introduce functional groups on the graphitic planes and that has been recently employed in the fabrication of elastomeric composites with improved mechanical properties [2]. In order to understand the mechanism beneath the interaction between the pyrrole and the substrate and thus the behavior of the functionalized filler, a more in-depth analysis is requested. A theoretical work based on molecular dynamics simulations and a DFT study were performed in order to investigate the interaction energy, the geometry of interaction and the mobility of N-substituted pyrrole molecules adsorbed on the graphene planes. This theoretical study at atomistic level can help design a new class of high-performance fillers by better understanding the interaction mechanism [3] given the important role of supramolecular interactions.

References

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