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Detailed atomistic simulations of functionalized graphene/polymer systems PETRA BACOVA, ANASTASSIA RISSANOU, Institute of Applied and Computational Mathematics (IACM), Foundation for Research and Technology Hellas (FORTH), GR-70013, Heraklion, Crete, Greece, VAGELIS HARMANDARIS, Department of Mathematics and Applied Mathematics, University of Crete, GR-70013, Heraklion, Crete, Greece — Graphene structures produced by the reduction of the graphene oxide contain some oxygen percentage coming mainly from the carboxyl groups remained on the edges of the graphene. With the increasing importance of the graphene in the material science, here we draw our attention to the effect of these groups on the properties of the graphene-based materials. Molecular simulations can be a valuable tool for the study of such complex materials at the molecular level. We have performed detailed atomistic simulations of hybrid nanostructured polymer/graphene materials for different polymer matrices. We study the behaviour of polymer nanocomposites with three types of dispersed graphene: (a) the pure non-functionalized sheet, (b) graphene with hydrogens grafted on the edges and (c) carboxyl-functionalized graphene. Data concerning the structural and dynamical properties of the polymer chains are presented. In addition, we compute the dynamic properties of the particular graphene sheets and we discuss in detail the importance of the strong electrostatic interactions present in the systems. The information obtained on the molecular scale in our work contributes to the understanding of the miscibility and the mechanical properties of the graphene/polymer nanocomposites.

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