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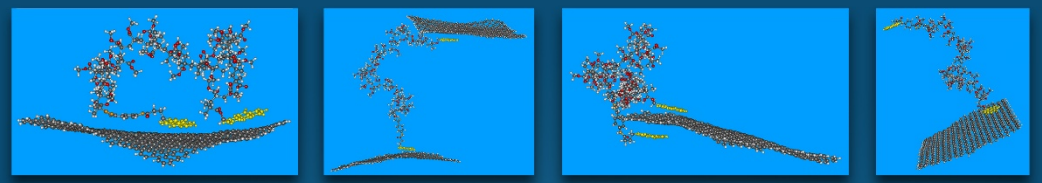

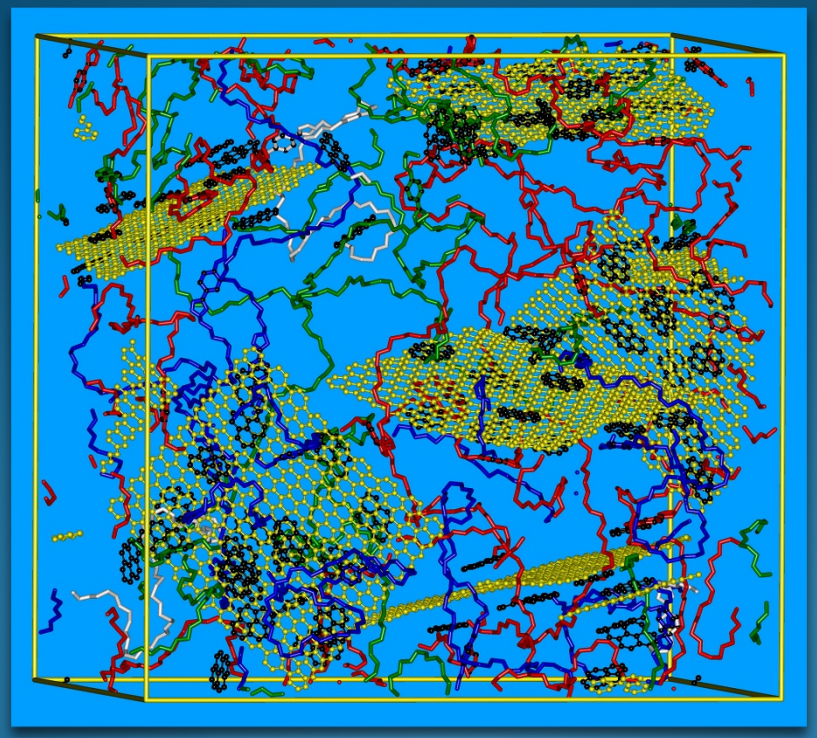

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About the Cover: Detailed, all-atom molecular dynamics simulation showing typical conformations of adsorbed Py-PMMA-Py chains on graphene sheets: loops (blue), bridges (red), dangling ends (green), and free chains (white).

"Molecular Modeling Combined with Advanced Chemistry for the Rational Design of Efficient Graphene Dispersing Agents"

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Abstract

Pyrene-functional PMMAs were prepared via ATRP-controlled polymerization and click reaction, as efficient dispersing agents for the exfoliation of few-layered graphene sheets (GS) in easily processable low boiling point chloroform. In parallel, detailed atomistic simulations showed fine dispersion of the GS/polymer hybrids in good agreement with the experiment. Moreover, the molecular dynamics simulations revealed interesting conformations (bridges, loops, dangling ends, free chains) of GS/polymer hybrids and allowed us to monitor their time evolution both in solution and in the polymer nanocomposite where the solvent molecules were replaced with PMMA chains. Microscopic information about these structures is very important for optimizing mechanical performance. It seems that the combination of atomistic simulation with advanced chemistry constitutes a powerful tool for the design of effective graphene dispersing agents that could be used for the production of graphene-based nanocomposites with tailor-made mechanical properties.

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