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## A Molecular Dynamics Study of the Interfacial Regions Between Polymer and Carbon-Based Nanoparticle Fillers

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A novel polymer composite material with high stiffness and thermal endurance can be designed by optimizing the filler content. We investigated the microscopic properties of the interfacial regions between cis-polyisoprene (natural rubber) and carbon-based fillers, e.g. fullerenes by using classical molecular dynamics (MD) simulations. The microscopic analysis shows that increasing filler concentration results in the growing of the regions containing ordered cis-PI chain at the interfacial areas. In this work, we analysed the order parameter, e.g. local density and orientation at the interfacial and confined regions which correspond to changes in mechanical and thermal properties. These results could provide the information for the parameterisation of the coarse-grained or the continuum models.

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