# A molecular dynamics study of non-covalent interactions between rubber and fullerenes

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**Abstract**
The percolation and networking of filler particles is an important issue in the field of rubber reinforcement, and much effort is given to clarify the true nature of the reinforcement mechanism and the viscoelastic behavior. The concentration of nano-fillers also in the presence of large amounts of carbon black is a parameter that can influence the macroscopic rubber behavior [1]. In this paper, non-covalent interactions between carbon $C_{60}$ fullerenes with poly-1,4-*cis*-isoprene, either as such or modified with a terminal carboxylate group are studied through atomistic simulation based on Molecular Mechanics (MM) and Molecular Dynamics (MD) methods. At first the conformational properties of a single chain and of twelve chains of poly-1,4-*cis*-isoprene, are studied. Afterwards, the conformational properties of a single chain of poly-1,4-*cis*-isoprene polymer terminated with a COOH group, and then a bulk system formed by chains of unmodified and some chains of modified poly-1,4-*cis*-isoprene in a periodic simulation box are simulated. Then, the systems formed by adding five $C_{60}$ fullerenes to the bulk systems of twelve poly-1,4-*cis*-isoprene chains, respectively containing either the unmodified polymer only, or the mixture of ten unmodified and two modified chains described before are atomistically modeled using simulation protocol in previous work proposed by Raffaini *et al*.[3]. The simulation results show relatively small interaction energy between rubber and fullerenes, the latter being well dispersed in the sample.The simulations showed a preferential tendency of fullerenes to display self-aggregation, in the presence of even a small fraction of modified polymer chains.

**References**
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