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Molecular Dynamics Simulation Of Novel Elastomer Nanocomposites: Structure Design And Property Prediction JUN LIU, LIQUN ZHANG, Beijing University of Chemical Technology — In this talk, by employing molecular dynamics simulation, we aim to provide the structure design and property prediction of novel elastomer nanocomposites(ENCs), by considering three typical systems such as physical compounding, self-assembly and end-linked systems. We examine the dispersion, interfacial interaction and the resulting static and dynamic mechanical properties of each system. Emphasis is placed on how to tune the visco-elasticity and decrease the dynamic hysteresis loss of ENCs, by considering to introduce the flexible nanoparticles(NPs) with reversible mechanical deformation such as carbon nanosprings and graphene nanoribbon, or by achieving a homogeneous distribution of NPs in the elastomeric polymer matrix together with decreasing the mobility of the end-groups of polymer chains. In particular, the end-linked system exhibits both excellent static and dynamic mechanical properties, independent of the temperature. This novel ENCs could provide some useful guidances for the fabrication of high performance ENCs tailored for tire tread of green tires by cutting the fuel consumption.

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