Progress in multi-scaled structure and related properties of elastomer nanocomposites explored by molecular dynamics simulation and experimental approaches

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In this talk I will systematically present some important simulated results of elastomer nanocomposites (ENCs) achieved via molecular dynamics simulation. First, we studied the dispersion and aggregation behavior of bare nanoparticles(NPs) with different geometries such as spherical, sheet-like and rod-like on the molecular scale. To model small ligands used in experiments to realize better dispersion, we investigated the dispersion of NPs end-grafted with polymer chains by varying the grafted chain length and grafting density. In addition, the effect of the middle- and end-functionalization on the dispersion of NPs is also covered. Second, we probed the translational and relaxation dynamics at the chain and segmental length scales of the interfacial regions, hoping to elucidate whether "glassy polymer layers" exist around NPs. Third, we simulated the enhancement of the stress-strain and fracture toughness induced by NPs, providing a molecular reinforcing mechanism. Fourth, the famous "Payne effect", namely the decrease of the storage modulus as a function of the strain amplitude was examined, uncovering the underlying reason responsible for this non-linear behavior, and meanwhile how the introduced carbon nano-springs can effectively reduce the dynamic hysteresis of ENCs is illustrated. Fifth, through simulation synthesis approach, we put forward a new and achievable approach to design and prepare a nanoparticle chemical network, with the NPs acting as "giant cross-linkers" or netpoints to chemically connect the dual end-groups of each polymer chain to form a network. We find this new network structure possesses excellent static and dynamic mechanical properties, highlighting a ultralow dynamic hysteresis loss tailored for green automobile tires. Computer simulation is shown to have the capability to obtain some fundamental understanding of ENCs, in hopes of providing some design basis and principles for synthesizing and fabricating multi-functional and high performance ENCs. In the meanwhile, I will show the preparation, structure-property relation and their industrialization of various high performance elastomer nanocomposites filled with clay, fibrillar silicate, silica, carbon nanotubes and graphene.

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Short CV

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