Research Colloquium

Title: Structured Interfaces of High-Performance Elastomers: Experimental and Computational Approaches

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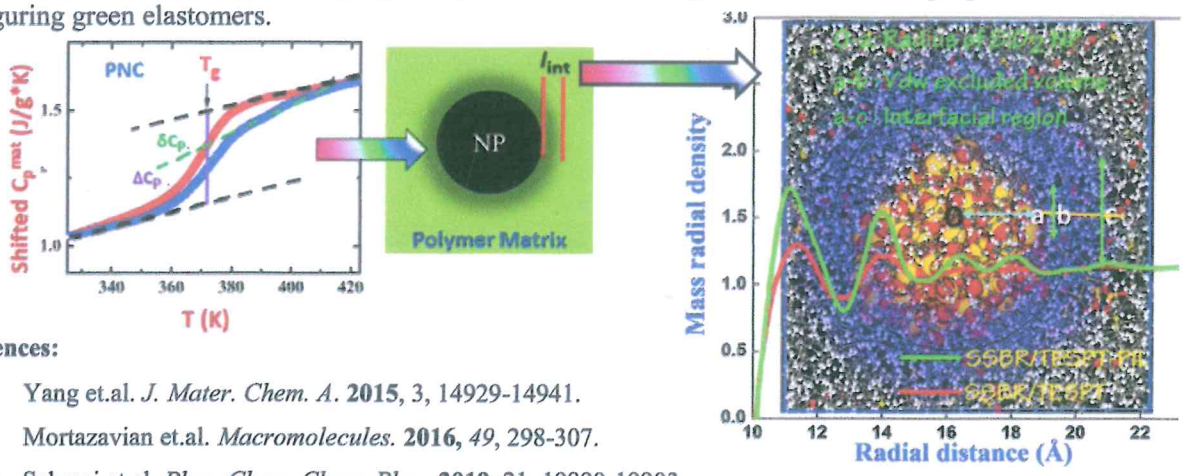
Speaker: Abdul Sattar Mohammad
Roll No: CY15D106

Venue: CB 310
Date: 17. 03. 2020
Time: 3.00 pm

Nanocomposites are fundamentally new class of materials in which the nanoparticles (NPs) induce interfacial reconstruction[1] via multiple non-covalent interactions culminating in varied material properties. While it is known that the properties of polymer nanocomposites (PNCs) are largely dominated by the interfacial layer around the nanoparticles, the molecular parameters controlling the interfacial layer structure and dynamics are complex and remain feebly studied[2,3]. This work provides an in-depth analysis of the interface structure and associated chain dynamics of the silica NP-filled Styrene-butadiene and Natural rubber PNCs at a scale close to the relevant molecular processes, directly correlating their micro/macroscopic properties[4,5] utilizing ionic and ionic liquid modifiers and cross-linkers. Accordingly, improved thermal stability, high-temperature shifts in the glass transition, the self-healing ability and the dynamic-mechanical performance of the PNCs were accrued from the existence of a strengthened and larger interfacial layer, tapped by systematic dielectric relaxation spectroscopy and temperature modulated differential scanning calorimetry. Specifically, the computed density and radial distribution profiles[6] from molecular dynamics simulations unraveled the structural configuration of the polymer chains with restricted dynamics, stabilized by specific intermolecular electrostatic, H-bonding and ion-dipole interactions at the polymer/silica NP interface. The designed hybrids exhibited improved viscoelastic properties towards configuring green elastomers.



References:

1. Yang et.al. *J. Mater. Chem. A.* **2015**, 3, 14929-14941.
2. Mortazavian et.al. *Macromolecules.* **2016**, *49*, 298-307.
3. Sahraei.et.al. *Phys. Chem. Chem. Phys.* **2019**, 21, 19890-19903
4. Abdul Sattar and A. Patnaik. *Soft Matter.* **2019**, *15*, 2826-2837
5. Abdul Sattar and A. Patnaik. *ACS Omega.* **2019**, *4*, 10939-10949.
6. Abdul Sattar and A. Patnaik, Communicated (**2020**).

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