Tailoring the Macroscopic Properties of Polymer Nanocomposites by Nanoparticles via Interfacial Engineering

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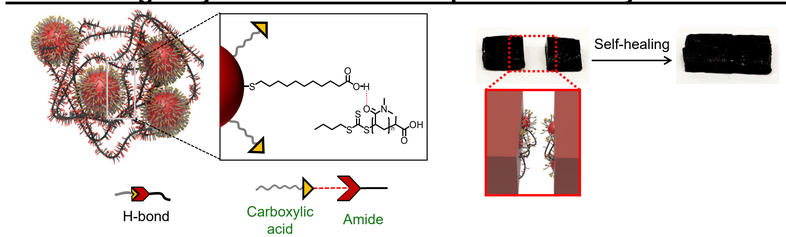
Abstract

Self-healing recyclable polymers are proposed as sustainable materials to mitigate waste associated with conventional plastics. Self-healing behavior can be introduced via the incorporation of surface-functionalized gold nanoparticles (AuNPs) into polymer matrices of poly(*N,N*-dimethyl acrylamide) (PDMA), however at the cost of a very stiff and brittle mechanical framework. This project addresses such trade-off by engineering enthalpic (hydrogen bond) and entropic (particle size) interactions at the nanoparticle-polymer interface. Control of nanoparticles via concentration, size (5-18 nm), and surface functionality along with the incorporation of soft polymer architecture of poly(butyl acrylate) (PBA) is shown to tailor thermal and mechanical properties while maintaining the healing rate. The results support the development of resilient, long-lasting materials by expanding their utilities into various demanding applications, ultimately contributing to waste reduction and environmental sustainability.

Background

Self-Healing Polymer Gold Nanocomposites with Dynamic H-Bonds



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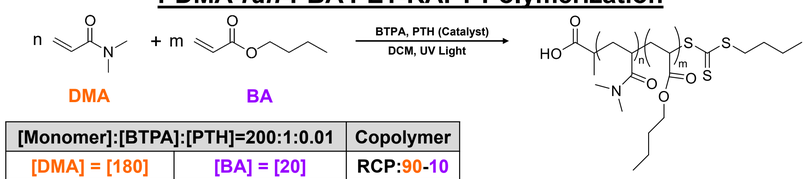
- Surface-functionalized AuNPs create particle-based crosslinks within a polymer matrix.
- Multiple hydrogen bonds at the nanoparticle-polymer interface promote cooperative binding behavior, resulting in an excellent self-healing mechanism.
- However, the rigid and brittle nature of the polymer matrix (PDMA) hinders its usage, where softness, elasticity and flexibility are crucial.

Hypothesis: The addition of soft segments into a polymer nanocomposite system will reduce the overall stiffness and brittleness and help to deeply understand nanoparticle-polymer interaction microscopically.

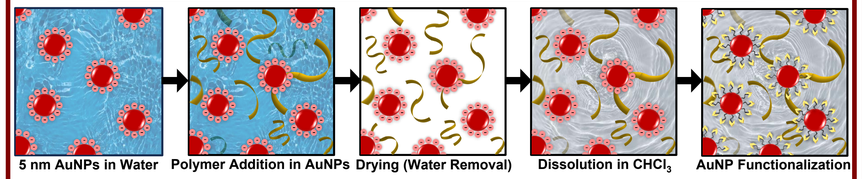
Methods

PDMA-*ran*-PBA PET-RAFT Polymerization



[Monomer]:[BTPA]:[PTH]=200:1:0.01		Copolymer
[DMA] = [180]	[BA] = [20]	RCP:90-10
[DMA] = [140]	[BA] = [60]	RCP:70-30
[DMA] = [100]	[BA] = [100]	RCP:50-50

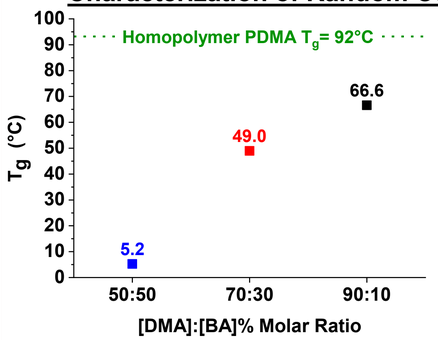
Synthesis of Polymer Gold Nanocomposites (AuNCs)

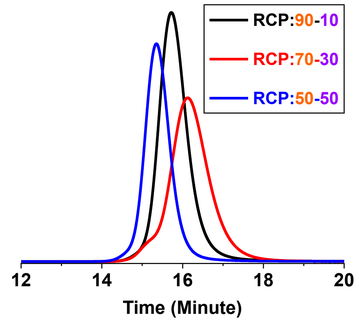


- All the samples were washed with hexane and dried overnight in the vacuum oven at 90 °C to remove moisture/solvent content.

Results / Discussions

Characterization of Random Copolymers with Range of T_g



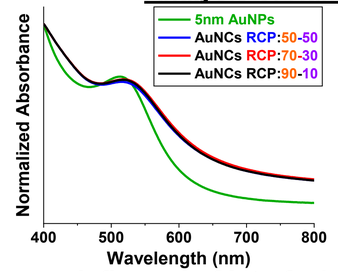


- Effects of **BA** chains on RCPs:
  - Softness and Elasticity increases.
  - Glass Transition Temperature (T_g) reduces with increment in relative **BA** proportion compared to **DMA.**

Copolymer	M_w	Dispersity (Đ)
RCP:90-10	21.9 kDa	1.14
RCP:70-30	17.3 kDa	1.20
RCP:50-50	22.9 kDa	1.11

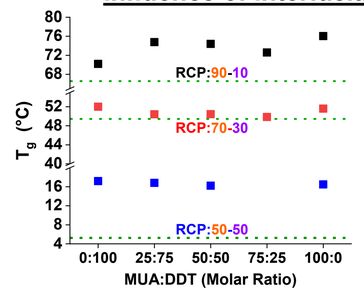
Results / Discussions

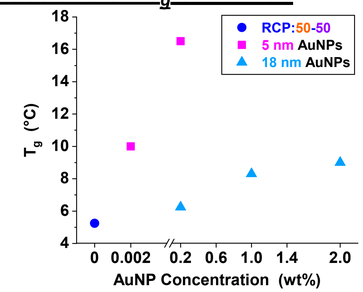
Analysis of Nanoparticles within AuNCs



- The size of nanoparticles within AuNCs after functionalization is verified by UV-vis spectroscopy.
- The absorbance peak around 516 nm indicates the nanoparticle diameter of approx. 5 nm without aggregation.

Influence of Interfacial Interactions on T_g of AuNCs





- **RCP:90-10**: Larger response in T_g through interfacial H-bonds
- **RCP:50-50**: Greater impact on T_g with smaller AuNP size

Conclusion & Future Research

- T_g / softness can be tailored by changing the relative ratio of [DMA]:[BA] into random copolymers.
- Functionalized AuNPs act as crosslinkers and Increase the T_g.
- Increasing the [DMA]:[BA] ratio of RCP in AuNCs leads to more dominant enthalpic interactions than entropic interactions.
- Future Work:
  - Mechanical test (*e.g.*, modulus & stress-relaxation).
  - Expand systematic study to RCP:60-40 and RCP:80-20.

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