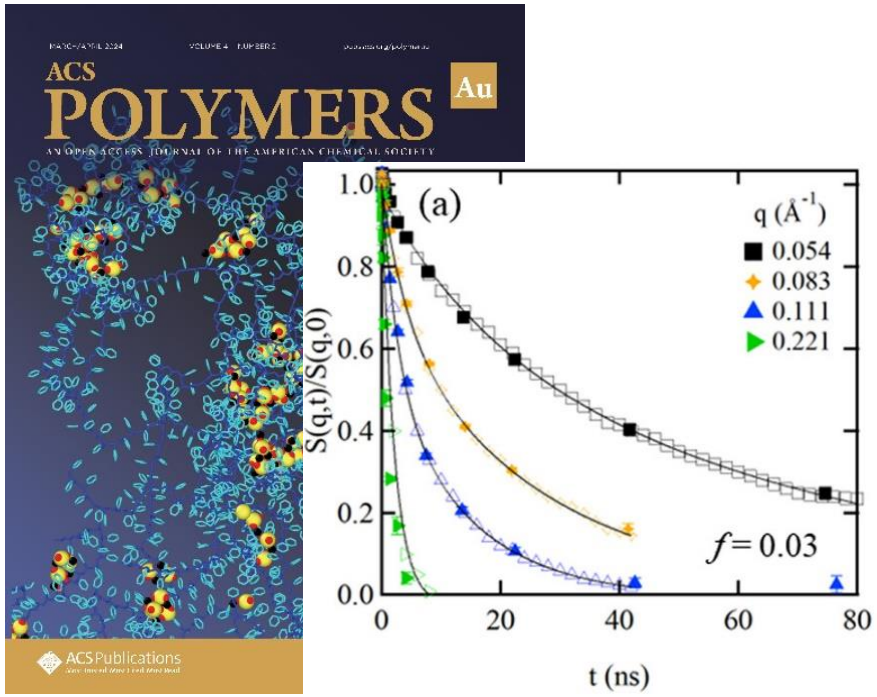
From Molecular Constraints to Macroscopic Dynamics in Associative Networks Formed by Ionizable Polymers



Visualization of sulfonated polystyrene ionomer in toluene. Sulfur (yellow), Oxygen (red), Na^+ (black), polystyrene backbone (blue) (left). Dynamic structure factor *S(q,t)* from NSE (filled) and atomistic MD simulations (open) showing the excellent agree between the two (right).

Kosgallana C.; Wijesinghe S.; Senanayake M.; Mohottalalage S. S.; Ohl, M.; Zolnierczuk, P., M.; Grest G. S.; Perahia D. "From Molecular Constraints to Macroscopic Dynamics in Associating Networks Formed by Ionizable Polymers: A Neutron Spin Echo and Molecular Dynamics Simulation Study," ACS Polymers Au 4, 149-156 (2024).

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Scientific Achievement

Neutron spin echo (NSE) and atomistic molecular dynamics (MD) simulations revealed multi-scale dynamics of networks formed by sulfonated polystyrene solutions that strongly depends on the size and distribution of the ionic clusters.

Significance and Impact

Resolving the multiscale dynamics of these networks directly impacts the processing of ionizable polymers. A feedback loop between NSE and MD simulations results provides a new effective approach to study soft materials.

Research Details

- NSE results for polystyrene sulfonate in toluene were analyzed by the sum of two exponentials, providing two distinctive dynamics time scales.
- Multimillion atomistic MD simulations generated computed networks for the same system. Dynamic structure factor is the same for the 2 methods with no adjustable parameters.