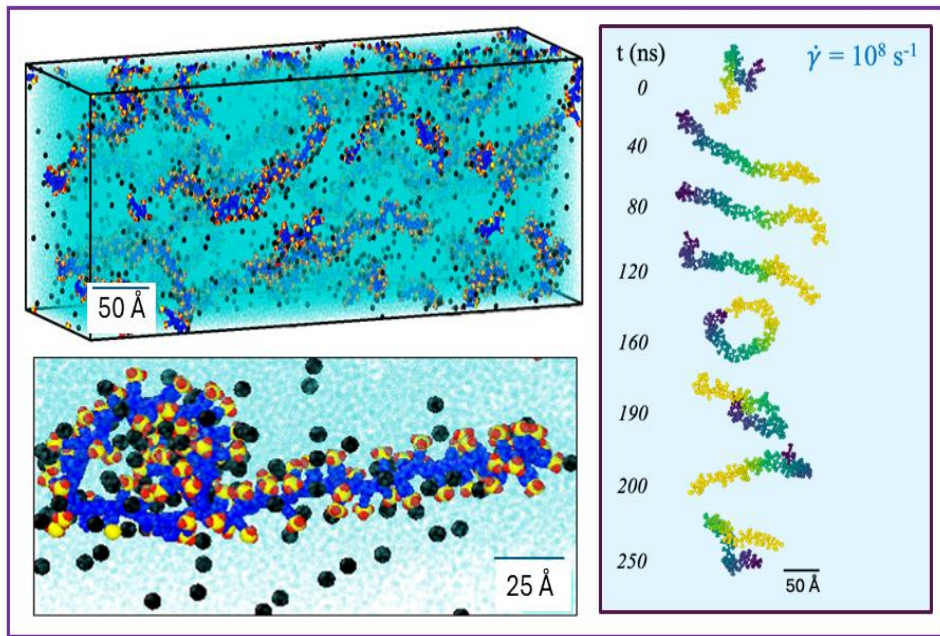


# Shear-Induced Conformations of Polyelectrolytes in Water: A Route to Effective Device Manufacturing

## Scientific Achievement

A CINT User Team investigated resolving polyelectrolytes shear-induced conformation fluctuations in water, including stretching and tumbling. The chain configuration is correlated with shear rate and degree of counterion condensation.



**Figure:** Visualizations of an aqueous solution of per-sulfonated polystyrene at a shear rate of  $10^8 \text{ s}^{-1}$  (Left). The polymer backbone is blue, sulfur yellow, oxygen red, sodium black, and water cyan. Right panel depicts one of the unique instabilities, tumbling, as a function of time, with the chain ends marked in different colors.

## Significance and Impact

Understanding the conformation instabilities under shear in aqueous polyelectrolyte solutions provides fundamental structural insights across time and length scales that directly affects their manufacturing pathways for integration into energy storage devices.

## Research Details

- Aqueous solutions of per-sulfonated polystyrene polyelectrolytes were studied by fully atomistic classical molecular dynamics simulations.
- Non-equilibrium molecular dynamics shear simulations were performed.
- Solution characteristics were extracted and correlated with shear rate.

Work was performed, in part, at the Center for Integrated Nanotechnologies.

Meedin, S.; Grest, G. S.; Perahia, D. Shear Response of Polyelectrolytes in Water. *Phys. Rev. E*. 2026.