

Diffusive dynamics of intrinsically disordered proteins in the condensed phase

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Biomolecular condensates formed by liquid-liquid phase separation organize cellular biochemistry, and alter their function. How fast molecules diffuse within the dense phase and how they responds to mechanical stress, governs both their biological function and their pathological aging. Resolving these properties from simulation is computationally demanding, the relevant dynamics are slow, the condensed phase is crowded, and converged transport and rheological observable require simultaneously large system sizes and long well-sampled trajectories. We use the Matini3 coarse-grained force-field to perform large-scale molecular dynamics, and investigated the diffusive and viscoelastic properties of intrinsically disordered protein called FUS. We find that molecules are experiencing confinement effects, lead to the sub-diffusive behavior, within the condensed phase. We further quantify the frequency-dependent viscoelastic moduli from stress-autocorrelation analysis, revealing crossover from viscous to elastic response.