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**Molecular Dynamics Simulations of the Fluctuating Conformational Dynamics of the Intrinsically Disordered Proteins $\alpha$-Synuclein and $\tau$** W. WENDELL SMITH, CARL SCHRECK, Department of Physics, Yale University, ABHINAV NATH, ELIZABETH RHOADES, Department of Molecular Biophysics and Biochemistry, Yale University, COREY O'HERN, Department of of Mechanical Engineering and Materials Science, Yale University — Intrinsically disordered proteins (IDPs) do not possess well-defined three-dimensional structures in solution under physiological conditions. We develop united-atom and coarse-grained Langevin dynamics simulations for the IDPs $\alpha$-synuclein and $\tau$ that include geometric,attractive hydrophobic, and screened electrostatic interactions and are calibrated to the inter-residue separations measured in recent smFRET experiments. We find that these IDPs have conformational statistics that are intermediate between random walk and collapsed globule behavior and demonstrate close resemblance to the known experimental data, with both electrostatics and hydrophobicity strongly influencing the dynamics. We investigate the propensity of $\alpha$-synuclein to aggregate and form oligomers, and present preliminary results for the aggregation of $\tau$ and interactions between these IDPs and small molecules such as heparin and spermine which are known to induce aggregation.

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