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Structural and Dynamical Characteristics of Polyelectrolyte Dendrimer Solutions Revealed by Neutron Scattering and Atomistic Simulation BIN WU, Oak Ridge National Laboratory, YUN LIU, National Institute of Standards and Technology, LIONEL PORCAR, PETER FALUS, Institut Laue-Langevin, CHANG-WOO DO, Oak Ridge National Laboratory, MICHALEA ZAMPONI, Forschungszentrum Julich, KUNLUN HONG, GREGORY SMITH, WEI-REN CHEN, Oak Ridge National Laboratory — Solutions of polyelectrolyte dendrimers were investigated using small angle neutron scattering (SANS) and dynamical measurements including quasi-elastic neutron scattering, neutron spin-echo and high resolution NMR. The goal of the experiments was to understand the structural and dynamical responsiveness polymer toward the variation of molecular charge. Experimental spatial correlation functions and temporal correlation functions such as intermediate scattering functions and the dynamic structure factor were evaluated quantitatively. Complementary atomistic simulations were developed for providing the microscopic interpretation of the scattering measurements and for investigating the material characteristics that are not accessible experimentally. Based on this synergistic approach, we attempt to provide a detailed understanding of the microscopic mechanisms underlying the observed electrostatic responsive properties in these very important classes of materials.

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