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TITLE

pH induced conformational change and intramolecular dynamics of PAMAM dendrimers

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Dendritic polymers-dendrimers-exhibit flexible conformations and complex dynamical behaviors in response to external stimuli. Consequently, understanding dendrimer structural evolution and dynamics as a function of environmental parameters presents the critical challenge to both experiments and theories.

We developed a novel quantum mechanics (QM) based atomistic force field (Dreiding III), in which the intermolecular parameters were optimized against QM calculations so that all potential key intermolecular interactions can be accurately described. This full atomistic force field permits the large-scale MD simulations on dendrimers with explicit solvent molecules and counterions. The accuracy of our MD simulations has been validated by the Small Angle Neutron Scattering (SANS) experiments: Upon increasing the molecular protonation, the predicted evolutions of radius of gyration (RG) and the molecular density profile of the PAMAM dendrimers agree quantitatively well with the SANS results.

The Neutron Spin Echo (NSE) experiments were recently done for generation 5 (G5) PAMAM dendrimers in aqueous solutions at various pH. The NSE experiment observed the pronounced peaks at high q ranges (1~2 nm^{-1}), indicating the strong intramolecular collective motions. We elucidate the origin of these collective motions theoretically by combining molecular dynamics (MD) and normal mode (NM) analysis, together with the neutron scattering theory. The normal modes with large collectivity and low frequency have most significant contributions to the effective diffusion coefficients, thus characterize the major domain motions of the dendrimers. Understanding the intrarmolecular dynamics of dendrimers is crucial to utilizing dendrimers as drug delivery vehicles in emerging nano-medicine.

Biography

Dr. Yi Liu obtained his Ph.D in Materials Science and Engineering from Institute of Metal Research, Chinese Academy of Sciences, P. R. China in 1997. Since then, he had been working as a postdoctoral fellow at Nagoya University, Japan (1997-2002), Forschungszentrum Jülich, Germany (2002-2003), and University of Western Ontario, Canada (2003-2005). In 2006 he joined Materials and Process Simulation Center at California Institute of Technology as a director of Computational Materials Design Facility. He has published more than 30 papers in peer-reviewed journals and served as an active referee for journals including Physical Review Letter/B/E and Journal of Physical Chemistry.