269e Polyhedral Oligomeric Sislesquioxanes in Solution: Insights from All-Atom Molecular Dynamics Simulations

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Polyhedral oligomeric silsesquioxanes (POSS) are considered building-blocks for novel organic-inorganic hybrid nanocomposite materials. While a rapidly increasing number of applications are being proposed for POSS-polymer systems, the molecular mechanisms that govern their thermodynamic and transport properties are, at present, not adequately understood. Molecular simulation is the ideal tool for investigating these mechanisms. We have performed molecular-dynamics simulations to study the properties of bare, octa-functionalized, polymer-tethered, and dumb-bell POSS monomers dissolved in liquid hexane, hexadecane, and poly(dimethyl siloxane). We report results for radial distribution functions, structural parameters (valence bond distributions, valence and dihedral angles), and self-diffusion coefficients over a wide temperature range. Our data are useful for developing coarse-grained models of POSS systems and for understanding the molecular mechanisms that determine the self association of POSS monomers to form supra-molecular structures. We will discuss these and the practical implications of our results.

Keywords: POSS, hexane, hexadecane, poly(dimethyl siloxane), radial distribution function, self-diffusion coefficient