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A Polyhedral Oligomeric Silsesquioxane-Polyoxometalate Hybrid Shape Amphiphile: Facile Synthesis, Characterization and Crystal Structure HAO LIU, JING WANG, KAN YUE, JING JIANG, WEN-BIN ZHANG, STEPHEN CHENG, Department of Polymer Science, The University of Akron —

This study contains the synthesis and characterization of a novel shape amphiphile composed of two covalently conjugated inorganic nanoparticles, i.e. an isobutyl substituted polyhedral oligomeric silsesquioxane (BPOSS) cage and a Lindqvist-type hexamolybdate ([Mo6O19]2-) cluster, and its crystal structure. The facile one-step coupling strategy was realized via the highly efficient palladium-catalyzed Sonogashira reaction between an alkyne-bearing POSS derivative (BPOSS-Alkyne) and an iodo-functionalized Lindqvist precursor (Lind-Iodide) in high yield. The precisely defined molecular structure was thoroughly characterized by combination of routine techniques, such as $_1$H and $_{13}$C NMR, FT-IR, and MALDI-TOF mass spectroscopy. The persistent shape and chemical incompatibility of the two building blocks, as well as the rigid *p*-phenylene ethynylene linker, drive BPOSS-Lind to pack into a monoclinic lattice, which was confirmed by bright field transmission electron microscopy (TEM), selected area electron diffraction (SAED), small angle X-ray scattering (SAXS) and wide angle X-ray scattering (WAXS). This work introduces a new dumbbell-shaped giant hybrid molecule (BPOSS-Lind) and shed light on the packing behavior of this shape amphiphile.

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