

PMSE 238

Shape-persistent polyphenylene-based dendrimers: A computational approach

Sabrina Pricl, Marco Ferrone, Maurizio Fermeglia, and Andrea Asquini. Department of Chemical Engineering, University of Trieste, Piazzale Europa 1, Trieste, 34127, Italy

Polyphenylenes dendrimers – 3D compounds containing benzene rings linked by sigma-bonds – form an increasingly important class of organic materials, as the benzene ring is an extremely flexible modulus for the construction of a wide range of structures and can bear a large range of active functionality. Also, the delocalized p-systems on adjacent rings can overlap to form extended conjugate systems. These peculiar structures may be used as scaffolds with a wide variety of functionality, enabling them to be used as functional nanoparticles with a vast range of possible applications. In this work we have performed a thorough characterization, by computer simulations, of the first three generation of three polyphenylene dendrimeric families, both underivatized and substituted with amino and carboxy groups in a solvated environment, with the purpose of studying the relevant structure-property relationships to be exploited in biomedical applications.

[Joint PMSE/POLY Poster Session](#)

[Sci-Mix](#)

[Division of Polymeric Materials: Science and Engineering](#)
[The 225th ACS National Meeting, New Orleans, LA, March 23-27, 2003](#)