Three-dimensional, nanosized phenylene-based dendrimers: scaling properties studied by a computational approach

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3D polyphenylene dendrimers can be prepared in ways that enable control of their shape, and their structures may be used as scaffolds with a wide variety of functionality, enabling them to be used as functional nanoparticles with a wide variety of possible applications, ranging from light emitting devices to biological sensors or drug delivery tools. As PDs have been synthesized only recently, their structural and chemico-physical characterization is still in its infancy. Accordingly, in this paper the shape and internal organization of three PD families based on three different cores were probed by accurate, atomistic molecular dynamics simulations (MD). Particular care was taken to ensure complete structural equilibration by implementing a MD simulated annealing protocol prior to evaluation of the molecular structure and dynamics. All dendrimer families were found to be characterized by molecular dimensions in the nano-range, and by a shape-persistent, non-spherical structure, of molecular fractal dimension around 2.5-2.6, and of surface fractal dimension practically constant and almost equal to 2 with increasing generations in all cases. The MD analysis revealed also that, for this type of dendrimers, the starburst limited generation is presumably located in correspondence of the third generation.