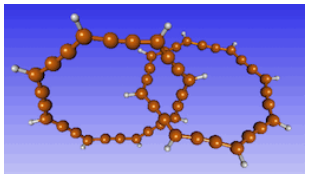
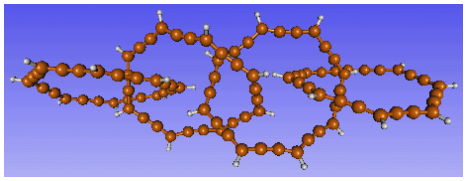
Interlocked cyclo[n]carbon rings

Ivan Cernusak

Department of Physical and Theoretical Chemistry, Faculty of Natural Sciences, Comenius University in Bratislava, Ilkovičova 6, 84215 Bratislava, Slovakia

Carbon fullerenes, nanotubes, rotaxanes, catenanes, knots, molecular motors – these and other large chemical compounds are paving the road to new materials. The idea of unconventional cyclic compounds – catenanes - was first envisaged by German chemist R. M. Willstätter in 1912 [1] and had been intriguing numerous chemists for many years. The long-lasting efforts in the quest for rotaxanes, catenanes and molecular motors resulted in the 2016 Nobel prize awarded to J.-P. Sauvage, J. F. Stoddart and B. L. Feringa. Carbon allotropes built from rings of two- or three-coordinate atoms – cyclo[n]carbons – represent another fascination and challenge to chemists because of their unique properties.

Recently, cyclo[n]carbon rings have been studied quite intensively [2-6]. In this contribution, we are attempting to look at catenane models based on cyclo[n]carbon rings from different perspective and present the results of computational experiments with the interlocked cyclo[n]carbon rings of various size and extent of interlocking. We have investigated both aromatic and anti-aromatic cyclo[n]carbon rings at the wB97XD level with the aim of showing how these building blocks can lead to "molecular threads" of different length. The very simple models of molecular threads are exposed to external force and the energy profiles of this stretching are presented.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