Routes to helicity

D. Chakrabarti, S. N. Fejer, and D. J. Wales

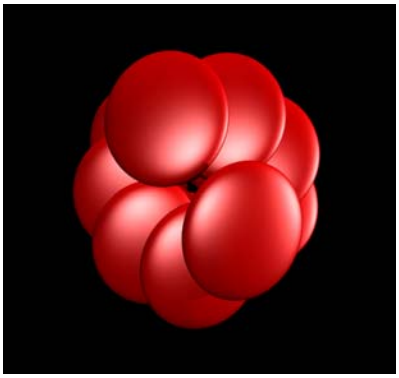
Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK

Self-assembly is nature's prescription for creation of complex structures from simpler building blocks. Adapting such a bottom-up approach is a potential route to fabrication of novel materials.[1] Here we demonstrate that nature can indeed guide us as we explore routes to helicity with achiral building blocks, driven by the existence of two competing length scales for intermolecular interactions, as in DNA.[2] To this end global optimisation studies of clusters bound by a variety of anisotropic pair potentials are first presented within a rigid-body framework[3]. We illustrate several realisations of helical architectures for clusters, the simplest one involving ellipsoids of revolution as building blocks.[4] In particular, we show that axially symmetric soft discoids can self-assemble into helical columnar arrangements. Finally, we describe the phase behaviour of these discoids in the bulk, focussing on the morphology of the columnar phase.[5] Understanding the molecular origin of such spatial organisation has important implications for the rational design of materials with useful optoelectronic applications.[6-8]

References

(1) S. Zhang, *Nature Biotechnol.* **2003**, *21*, 1171.
(2) J. D. Watson and F. H. C. Crick, *Nature* **1953**, *171*, 737.
(3) D. Chakrabarti and D. J. Wales, *Phys. Chem. Chem. Phys.* **2009**, in press.
(4) D. Chakrabarti, S. N. Fejer, and D. J. Wales (manuscript in preparation).
(5) D. Chakrabarti and D. J. Wales, *Phys. Rev. Lett.* **2008**, *100*, 127801.
(6) D. Adam, *et al. Nature* **1994**, *371*, 141.
(7) L. Schmidt-Mende, *et al. Science* **2001**, *293*, 1119.
(8) V. Percec, *et al. Nature* **2002**, *419*, 384.

Figure



Global minimum for a cluster of 13 axially symmetric discoids bound by a soft elliptic pair potential.