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Publisher *Taylor & Francis*

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## **Molecular Simulation**

Publication details, including instructions for authors and subscription information:

<http://www.informaworld.com/smpp/title~content=t713644482>

## **Guest editorial**

D. M. Heyes

**To cite this Article** Heyes, D. M.(2005) 'Guest editorial', *Molecular Simulation*, 31: 13, 865

**To link to this Article:** DOI: 10.1080/08927020500314043

**URL:** <http://dx.doi.org/10.1080/08927020500314043>

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## Guest editorial

D. M. HEYES

An auxetic material is one that dilates laterally when it is stretched, and conversely contracts when it is compressed. There are a number of naturally occurring materials exhibiting this counter-intuitive behaviour, including a number in the living world (as usual, Nature gets there first). The effect originates from a concerted and coupled response of the members used in construction. Auxetic materials are interesting both for their novelty and the many uses to which they can be put.

Since the late 1980s a range of synthetic auxetic materials has been constructed from, for example, composites, foams, and micro-porous polymers. These are perhaps best referred to as 'constructions' and 'structures'. The progress made in the field in the last two decades has been immense. Nevertheless, a significant challenge remains in how best to design and synthesise materials where this property originates at the molecular level, which this Special Issue addresses.

The importance of this subject has been recognised in the UK with the establishment of the Auxetic Materials Network, 'AUXNET'. An international workshop on 'Auxetics and Related Systems' was held in Będłow near Poznań, Poland in June 2004, which brought together

researchers from many countries and disciplines. This meeting inspired this Special Issue. Although there is significant literature already in this field, some of the fundamental issues leading to auxeticity still need to be established. For molecular-based auxetics, molecular simulation is proving an invaluable tool in this respect, as the articles in this issue demonstrate.

This Special Issue contains papers which cover the fundamental requirements for auxeticity, as well as articles dealing with the molecular modelling of generic and specific systems, both inorganic and organic in composition. Many of the papers are collaborations between different groups. This issue is groundbreaking in being entirely devoted to theoretical and simulation papers, providing a snapshot of the breadth and depth of current activity in the field. It surveys the work being carried out, the present state of knowledge and highlights areas where there still remain uncertainties and challenges.

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