New Directions of Research in Molecules and Materials

Foreword

'Materials' has emerged as a unifying theme of several traditional scientific disciplines. Reflecting this trend, this special issue of the *Journal of Chemical Sciences* is being brought out to coincide with an international conference on 'Molecules and Materials: New Directions', being held in Bangalore from 4 to 6 December 2008 and includes contributions from many of its participants.

The subject areas dealt with in this Issue are metal nanoparticles, carbon nanotubes, molecular materials, oxides and thin films. Ganguli *et al* (page 521–528) correlate properties of nano-structured materials with their molecular constituents. Sadhu and Patra (page 557–564) are interested in tuning optical properties by synthetic modifications, which they demonstrate with the $Cd_xZn_{1-x}S$ system. Thomas *et al* (page 529–536) use phosphomolybdates as the molecular constituents to derive nanostructured materials. While extended solids are discussed in the above papers, the paper by Das *et al* (page 547–555) deals with assemblies of nanoparticles with molecular linkers. Kulkarni *et al* (page 637–643) present a method to control the wetting behaviour of films grown at interfaces. Surfactant molecules can act as both reducing and capping agents as shown by Kasture *et al* (page 515–520) in the formation of silver nanoparticles. Although synthesis is important, properties of materials have been investigated by a number of researchers. While Khanuja *et al* (page 573–578) are interested in hydrogenation properties, Datta *et al* (page 579–586) probe the antibacterial effects and Medda *et al* (page 565–572) tune optical absorption. Solution phase chemistry is a central aspect of materials as demonstrated by Panchakarla and Govindaraj (page 607–611) in making dispersions of double-walled carbon nanotubes. Rajkumar and Ranga Rao (page 587–594) use ionic liquids as media to make materials. Kakade *et al* (page 599–606) report near complete phase-transfer of single-wall carbon nanotubes by covalent functionalisation. Bhat and Maitra (page 507–513) have shown that gold and silver nanoparticles, stabilized by bile-acid derived thiol-capping, self-assemble in aqueous solvents because of the amphiphilic nature of the capping agent.

Atomistic simulations are necessary to understand properties of materials. This is brought out well by Imam *et al* (page 621–626) who study the mechanisms of intermixing of Co and Ag on Rh(111) surface. The structural details probed by diffraction can give new interpretation for hydrogen bonding as well as properties such as dipole moments, as shown by Reji Thomas *et al* (page 613–620). Atomistic modelling can give new insights into the design of novel sensors; for example, the mechanism of action of an arsenic sensor is unraveled by Mallajosyula *et al* (page 627–635). Changes at the atomic scale affect bulk properties such as magnetism and a correlation between the two is evident in the work of Madhu and Sundaresan (page 595–598). Molecular changes occurring at the nanoscale are of great interest as shown by Rajeev Kumar *et al* (page 537–546) in the study of alkyl chain dynamics in metal nanoparticles.

We hope that this special issue will be welcomed by the Chemical Sciences fraternity, especially by those engaged in research on various aspects of materials.

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