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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>

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To cite this Article Pettitt, B. M.(2006) 'Guest editorial: Nanobiology', *Molecular Simulation*, 32: 10, 773

To link to this Article: DOI: 10.1080/08927020601009989

URL: <http://dx.doi.org/10.1080/08927020601009989>

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Guest editorial: Nanobiology

Nanotechnology and biology are merging to form nanobiology. This field is emerging from a convergence of tools and methods in surface science, synthesis and biology. The emphasis that distinguishes nanobiology from related fields emphasis is on living systems and biomaterials at the nanoscale level. Nanoscale structures and properties are increasingly important. Biological molecules acquire unique properties when used in conjunction with other nanoscale structures and patterns. At the nanoscale level, natural and manmade nanoscale systems are not well described by simple extrapolation of molecular or macroscopic phenomena. As a result, new structural, computational and chemical tools have been developed by nanoscientists to address specifically the unique material properties in these systems not easily captured through conventional analysis.

Nanobiology, thus formulated, does not displace traditional biochemistry, since many systems can be described using conventional molecular tools; instead, this emerging discipline focuses on the properties and structure of complex assemblies of biomolecules, such as biochips, molecular motors and membrane assemblies in conjunction with the distinctive surfaces, rods, dots and materials of nanoscience. Conversely, the constructed materials of nanobiology cannot be described simply as molecules.

The convergence of these diverse fields is particularly timely. Global attention in nanoscience and biology is increasingly focused on organized assemblies at the nanometer scale. Biochemistry and chemistry have

progressed *up* to the study of macromolecular assemblies from the study of individual molecules. Through advances in nanofabrication, physics, engineering and materials science have concomitantly moved *down* to this scale from bulk processes. These trends intersect at the nanometer scale taking on a physical form often referred to as the “wet/dry” interface by our late colleague Rick Smalley.

Special theoretical and computational techniques are required to deal with these systems. Often times we find the systems are inhomogeneous. In addition, the size of the systems can be considerably larger in number of atoms than traditional studies of biochemical systems. However, we often find that the scale and homogeneity are not sufficient to allow for full mesoscale decimation of molecular details.

In this special issue of *Molecular Simulation*, papers were invited to demonstrate both the range of applications as well as the required techniques needed for nanobiology. There are no clear lines between this area and many other related fields like nanotechnology, biochemistry etc. We start with methods and move to applications. Each drive the other. The hope is that the papers here will give the reader a feel for the breadth of the field and a snapshot of the state of the art in this area.

B. M. Pettitt
Guest Editor
Houston, TX, USA, 2006