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Modelling of interfaces for biomedical devices: challenges ahead

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Abstract

Biointerfaces exist between inorganic materials and biological matter such as lipid bilayers, peptides and/or proteins, in the presence of water. There is a pressing need for clear understanding of the structure, bonding and dynamics of such hard/soft biointerfaces, particularly from the atomistic to mesoscopic scale. Such understanding is a prerequisite for design of materials with improved biocompatibility, biorecognition or biofunctionality, e.g. for implants, biosensors and bioelectronics, and for biomimetic synthesis of inorganic nanostructures. Medical implants support a continuously expanding industry, currently around £60billion/year. Unsatisfactory implant life often exists due to poor interface compatibility. Riding the tide of the bionanotechnology revolution, biosensors & DNA chips (array sensors) are creating an emerging market, with an estimated growth of over 40% per year. Future sensing arrays promise to address even more “down-stream” components in cell-cell communication processes (“cellomics”), where immobilization of peptides & proteins on (patterned) surfaces is critical to achieve biosensing and medical diagnostic functions. Bioelectronics is still at the explorative R&D stage but is likely to gain a substantial market share in 5-10 years. It takes advantage of Nature’s own methods of information storage & processing at the cellular level, where the primary building blocks are networks of real cells, or at the molecular level, where the building blocks are peptides, proteins and DNA strings. In both cases, the biological components need to be steered into a suitable pattern in or on an engineered surface, providing chemical/electrical I/O communication. On the other hand, biointerfaces are also important in non-biomaterials applications, e.g. in novel biomimetic synthesis, where the specific binding selectivity of peptides to metals/oxides has been steered to assemble inorganic nanostructures with novel electronic, optical, & magnetic propertie. Hence, biointerfaces underpin a number of new / emerging bio- and/or nano- technologies, of great potential for scientific discovery and technical exploitation. This presentation highlights the key issues and challenges for the investigation of biointerfaces from both experimental and theoretical points of view. Limitations in experimental characterisation further demand accurate simulative tools using purposely defined force field to probe into the molecular behaviour at specific inorganic surfaces.