COMPUTER MODELLING AS A TOOL IN MATERIALS SCIENCE

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We will describe how the use of modelling techniques especially in conjunction with a range of experimental methods can yield unique information on structures, dynamics and mechanism in a range of functional materials. Our discussion will concentrate on the following topics and systems

(i) Structure modelling and prediction of both inorganic and organic materials
(ii) Modelling of the structures and properties of oxide surfaces
(iii) Modelling of defect structures and properties, especially of wide band-gap semi-conductors
(iv) Modelling of nano-particle structures and properties
(v) Elucidation of the electronic structure and band alignment of titania polymorphs
(vi) Modelling of the mechanisms of catalytic reactions

We will discuss the future prospects of the field in the light of developments in computer hardware, methodologies and algorithms.