

Computer Modelling as a Tool in the Chemistry of Materials

Richard Catlow, Department of Chemistry, University College London

Computer modelling techniques are now used very widely in chemical, physical and biological sciences, especially in understanding the behaviour of complex systems at the molecular level. This lecture will highlight their application to materials chemistry where the impact has been substantial in recent years. Special emphasis will be given to three important and topical areas:

- Crystal structure prediction
- Guiding and understanding synthesis
- Modelling nucleation and growth
- Understanding reactivity at the molecular level

Applications to oxides, microporous silicates sulphides and molecular crystal will be discussed. Future prospects and developments in the field will be considered.