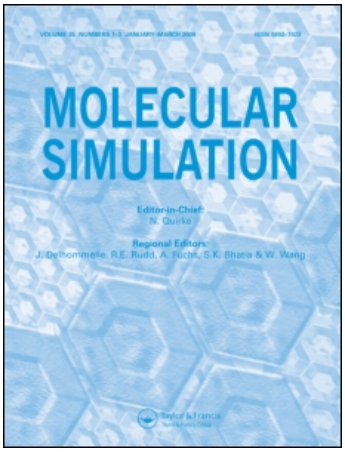

Molecular Simulation
Publication details, including instructions for authors and subscription information:
http://www.informaworld.com/smpp/title~content=t713644482

Guest Editorial

C. R. A. Catlow[a]
[a] The Royal Institution of Great Britain,

To cite this Article Catlow, C. R. A.(1994) 'Guest Editorial', Molecular Simulation, 12: 2, 75
To link to this Article: DOI: 10.1080/08927029408022524
URL: http://dx.doi.org/10.1080/08927029408022524

Molecular Simulation, 1994, Vol. 12, p. 75
Reprints available directly from the publisher
Photocopying permitted by license only

GUEST EDITORIAL

The discovery by Bednorz and Muller in 1986 of the phenomenon of high temperature superconductivity in oxides is the most significant event in the recent history of materials science. It led to an explosive growth in the study of the properties of mixed metal oxides, with new and higher temperature superconductors being synthesised within months of the original discovery. As the field of high T_c superconductivity has matured it has become clear that matters relating to defect structure, non-stoichiometry, the rôle of dopants and of oxygen ordering and diffusivity are crucial in influencing T_c. In addition surface and interfacial structures and properties are of vital importance in these materials. All these aspects of the solid state chemistry and physics of the high T_c oxides are amenable to study by computer simulation techniques. Indeed, the complexity of the problems is such that reliable simulations are an essential tool in constructing detailed models of the behaviour of the materials.

The six articles collected in this issue provide an illustration of the use of computer simulation in this field. Different applications of lattice statics, molecular dynamics and Monte Carlo methodologies are described; and the rôle of embedded quantum cluster calculations - an important technique in the study of many materials problems - is considered. The range and scope of the calculations described is typical of that in contemporary studies of ceramic oxides.

C.R.A. CATLOW
The Royal Institution of Great Britain