

COMPUTATIONAL MODELLING of OXIDES: BULK and SURFACE PROPERTIES

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We will first introduce both the role of modelling techniques in materials chemistry and will discuss briefly the nature of the bonding and cohesion in metal oxides. We will then focus on modelling and prediction of the bulk and surface properties of oxides. We will summarise the main techniques used and describe the present state-of-the-art by reference to transition metal oxide, silicate and aluminosilicate materials. Our account of surface structures will pay special attention to the problems raised by polar surfaces, which we will illustrate by reference to the widely studied surface chemistry of zinc oxide.

We will then address prediction of the structures of oxide nano-clusters, which again pose intriguing problems; and we will describe briefly the simulation of structures of glassy oxide.

We will conclude by discussing the prospects of the field in the light of developments in computer hardware, methodologies and algorithms.