

MS03.06.03 CALCULATION AND PREDICATION OF MOLECULAR STRUCTURES. Martin U. Schmidt.

MS03.06.04 MODELING MATERIALS WITH SYMMETRY. Christoph M. Koelmeel, 9685 Scranton Road, San Diego, CA 92121

State of the art computer aided modeling of solid materials can assist in all aspects of structure building, visualization, and determination. The efficiency of computational algorithms to tackle these problems increases substantially when symmetry information can be included. For example, the set of atoms within the asymmetric unit is sufficient to describe the complete crystal structure. In consequence, employment of spacegroup symmetry, symmetry visualization and automated symmetry detection form an important component of a state of the art solid state modeling environment. The presentation describes typical application scenarios that exploit symmetry tools and outlines the algorithms behind the recognition of three-dimensional translational and rotational symmetry.

MS03.06.05 FIRST PRINCIPLES SIMULATION OF OXIDE MATERIALS. Nicholas M. Harrison, Daresbury Laboratory, Daresbury, Warrington WA4 4AD, UK

The simulation of the physical and electronic structure of oxide materials within Hartree-Fock, density functional and hybrid methodologies will be described. Details of recent applications to the effect of defect structures on the properties of both simple and transition metal oxides will be presented.

MS03.06.06 COMPUTER MODELLING OF DEFECTS IN INORGANIC MATERIALS. Robert A Jackson, Chemistry Department, Keele University, Keele, Staffs ST5 5BG, UK

The use of computer modelling methods to study defects in inorganic materials is now well-established. The methods used will be reviewed, and recent applications considered as examples. In cases where the concentration of defects is low, defects may be modelled using techniques based on Mott-Littleton methodology. This approach models point defects or defect clusters as if they are at the centre of an otherwise perfect lattice, and uses continuum methods to represent the response of more distant regions of the lattice to the presence of the defect. The approach will be illustrated by a recent study on modelling divalent impurity ions in BaLiF_3 - a system with applications in laser devices.

Higher concentrations of defects may be modelled using supercell methods, in which the defects are included as part of a large unit cell or supercell. This enables defect-defect interactions to be taken into account explicitly, and also has the advantage that all lattice properties normally calculated by lattice energy minimisation can be obtained for the defective system. The approach has been used in a study of the $\text{UO}_2\text{-PuO}_2$ nuclear fuel, which will be given as an example.

PS03.06.07 MODIFICATION OF FINNIS-SINCLAIR POTENTIAL TO ACCOUNT FOR SURFACE EFFECT. Z. Kaszukur, Institute of Physical Chemistry PAS, Kasprzaka 44/52, 01-224 Warsaw, Poland

Long range N-body Finnis-Sinclair (F-S) potentials are the example of a simple tight binding approach to describe cohesion in transition and noble metals [1]. This approach applied to fcc transition metals describes satisfactory their elastic properties as well as direction of a surface driven relaxations, contrary to binary, Lennard-Jones type potentials [2]. The simple tight binding scheme is however far from accurate when predicting surface energy and leaves surface tension values underestimated by about 50% in comparison to experimental data. In the present work the surface tension values for 100, 110 and 111 surfaces have been calculated for F-S potentials for palladium evidencing similar discrepancy between the model and experiment. Calculated depth profiles of surface layers displacement show however excellent agreement with the experiment.

The problem of wrong energy estimation in the surface area may be cured by modifying the constant weighting the cohesive part of the simple tight binding potential, making it dependent on the local coordination number, when the interaction is restricted to nearest neighbours only [3]. A similar approach has been applied in this work to the long range F-S potentials after redefining the concept of the coordination number. The results of calculations for single crystal and cluster surface relaxation calculations is presented and discussed.

[1] A.P.Sutton, J.Chen, *Phil.Mag.Lett.*, **61**, 139-146 (1990).

[2] V.Rosato, M.Guillope, B.Legrand, *Phil.Mag.A*, **59**, 321-336 (1989).

[3] J.L.Rousset, J.C.Bertolini, P.Miege, *J.Phys.Chem.*, in print

PS03.06.08 "AKIRA", AN EXPERT SYSTEM TO PREDICT CRYSTAL STRUCTURES. Masahiko Hosoya, Hiroya Chinen and Makoto Nakamoto, Department of Physics, University of the Ryukyus, Japan

An AI (Artificial Intelligence) program is presented to predict crystal structures from the constituent atoms with no quantum mechanical calculation but the help of empirical laws. The program "AKIRA" made on an expert shell now only adopts a very few rules such as Hume-Rothery's one, preference of close-packed structures, Grymm-Sommerfeld's law, but gives correct answers to a fairly large fraction of the known crystals of type AB. The possibility of its expansion brightens its future practical usefulness just as its name "AKIRA" means brilliance like stars or crystals.