INFLUENCE OF OXYGEN VACANCIES AND 26 D-IMPURITY ON ELECTRONIC AND TRANSPORT PROPERTIES OF ZIRCONIA

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In this paper we have described a possible theoretical approach to the problem of the influence impurity on transport properties zirconia using molecular-orbital techniques. As examples we have treated D-elements and the oxygen vacancy in zirconia in some detail. In these examples we have used the simplest representation of molecular-orbital theory. The examples given were ones in which comparison with experiment could be made. This is an important role of theory – to make contact with and explain experimental results. Another important role of theory is to be able to supply insight and guidance in areas where no experimental information exists.

The present work is dedicated to the simulation of the electronic structure of 26 impurity d-elements (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Y, Nb, Mo, Tc, Ru, Rh, Pd, Ag, Lu, Hf, Ta, W, Re, Os, Ir, Pt, Au) and transport properties of zirconia using the tight-binding theory. The problems of this have been considered in the framework of the cell method and the band calculations.

The system is treated as a large molecule. The energy levels and wave functions for a cell are received with the help of molecular-orbital treatment. The received wave functions have precise physical interpretation in a sense of a degree of localization of a charge. For calculations of energy levels of cubic zirconia in the absence of a defect, we have the used a cell of 12 atoms, inclusive the 8 oxygen atoms and 4 zirconium atoms. We have considered electronic properties calculated for a group of atoms of dioxide, when one cation site is replaced with impurity atom and one anion is absent and nearest neighbour atom O moved along impurity to vacant site.

During simulation the impurity is placed in the substitutional site of zirconium. The calculations have shown, that the oxygen vacancy in zirconia is split-vacancy. We have established, that the migration barrier for oxygen in zirconia sharply decries at Cu, Ag, Ni, Pd, Pt and Au- doping.