



Abstract

Electronic structure of tin oxides

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Stannic oxide SnO₂ is a technologically important material which is frequently obtained by the oxidation of SnO. The tin oxides both have a tetragonal structure which differ essentially by the insertion of an oxygen plane between two tin planes in the layered SnO crystal. In order to well understand this structural evolution, it is crucial to have a precise description of the atomic and electronic structure of the two oxides. Preliminary results of calculations performed within Density Functional Theory in the Local Density Approximation (DFT-LDA) have already shown the relation existing between the electronic and geometric configurations of the two oxides [1]. The gap calculated for SnO₂ was in good agreement with the experimental value [2], but the calculations did not reproduce with a very good accuracy the experimental structure of SnO [1].

We present an *ab-initio* (DFT-LDA) study of the electronic structure of SnO, in comparison with SnO₂. The charge density distribution of each oxide is analysed with a special emphasis on low-charge-density contributions. Particular problems in the calculation of the equilibrium structure due to the pseudopotential of tin are put into evidence. We discuss the origin of these problems, and a possible solution. © 1999 Elsevier Science B.V. All rights reserved.

References

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