World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:8, No:02, 2014

Electronic States at SnO/SnO2 Heterointerfaces

Authors : A. Albar, U. Schwingenschlogel

Abstract : Device applications of transparent conducting oxides require a thorough understanding of the physical and chemical properties of the involved interfaces. We use ab-initio calculations within density functional theory to investigate the electronic states at the SnO/SnO2 hetero-interface. Tin dioxide and monoxide are transparent materials with high n-type and p-type mobilities, respectively. This work aims at exploring the modifications of the electronic states, in particular the charge transfer, in the vicinity of the hetero-interface. The (110) interface is modeled by a super-cell approach in order to minimize the mismatch between the lattice parameters of the two compounds. We discuss the electronic density of states as a function of the distance to the interface.

Keywords : density of states, ab-initio calculations, interface states, charge transfer
Conference Title : ICCECM 2014 : International Conference on Computational and Experimental Condensed Matter
Conference Location : Barcelona, Spain
Conference Dates : February 27-28, 2014