Arwa Albar et al., J Material Sci Eng 2017, 6:6(Suppl)
DOI: 10.4172/2169-0022-C1-077

Polar catastrophe at the MgO(100)/SnO_2(110) interface

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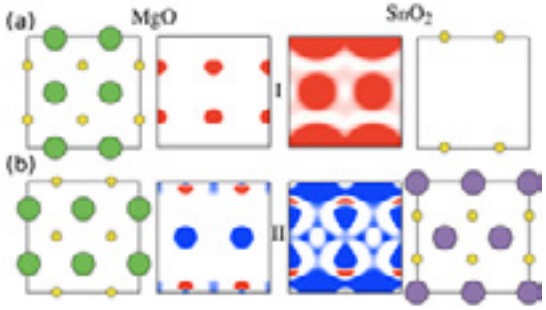
First principles calculations, based on density functional theory, are used to investigate the structural and electronic properties of the epitaxial MgO(100)/SnO_2(110) interface of wide band gap insulators. Depending on the interface termination, nonmagnetic metallic and half-metallic interface states are observed. The formation of these states is explained by a polar catastrophe model for nonpolar–polar interfaces. Strong lattice distortions and buckling develop in SnO_2, which influence the interface properties as the charge discontinuity is partially screened. Already a single unit cell of SnO_2 is sufficient to drive the polar catastrophe scenario.



Biography

In April 2017, Dr. Arwa Albar earned her Ph.D degree in Material Science and Engineering from King Abdullah University of Science and Technology, Saudi Arabia. Her research is based on Density functional theory calculation that is used to investigate the electronic, magnetic, and structural properties of oxide materials under defects and interfaces. She is also a staff in the Physics Department of King AbdulAziz University since 2004.

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