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Electronic properties and stabilities of bulk, nano-cluster, and low-index surfaces of SnO in comparison with SnO_2: application to high-temperature gas sensor YUHUA DUAN, National Energy Technology Lab — High-temperature gas sensors to detect various components of the gas flow in gasification technologies are highly desired. As one kind of the wide band-gap oxide semiconductors, tin oxides (SnO_2, SnO) are widely used as solid state sensor material, oxidation catalyst and transparent conductor. Due to the electronic structure and possibility of two different oxidation states of Sn^{4+} and Sn^{2+} and high thermal stability, tin oxides are very sensitive to oxidizing and reducing many kinds of gases, and therefore can be used to detect these gases with good sensitivity at high-temperature. In this study, based on density functional theory approach with an empirical correction of van der Waals interactions, the structural and electronic properties of the bulk, nano-cluster, and low-index surfaces of SnO_2 and SnO are obtained. Our results indicate that the differences between SnO_2 and SnO are significant and the convertible transition of $Sn^{4+} \leftrightarrow Sn^{2+}$ may have a great application in high-temperature sensor technology. In SnO, the van der Waals interactions play an important rule and may lead to more active sites for interacting with other molecules. By investigating the interactions between gas molecules (such as CO_2, C_2H_6, C_2H_5, *etc.*) with the surfaces of SnO_2 and SnO, the sensing mechanism of tin oxides will be explored.

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