

Abstract Submitted
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Effects of interlayer Sn-Sn lone pair interaction on the band gap of bulk and nanosheet SnO¹ NAOTO UMEZAWA, Natl Inst for Materials Sci, WEI ZHOU, Tianjin University — Effects of interlayer lone-pair interactions on the electronic structure of SnO are firstly explored by the density-functional theory. Our comprehensive study reveals that the band gap of SnO opens as increase in the interlayer Sn-Sn distance. The effect is rationalized by the character of band edges which consists of bonding and anti-bonding states from interlayer lone pair interactions. The band edges for several nanosheets and strained double-layer SnO are estimated. We conclude that the double-layer SnO is a promising material for visible-light driven photocatalyst for hydrogen evolution.

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