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Modulation of band gap in SnO by controlling interlayer Sn-Sn lone pair interaction

Wei Zhou[1], ○Naoto Umezawa[2,3] (1.Tianjin University , 2.NIMS, 3.PRESTO)

E-mail: umezawa.naoto@nims.go.jp

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.