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Ab Initio Study of Photocatalytic Activity of MIn2O4 (M = Ca, Sr) MASAHIKO KATAGIRI, TAIZO SASAKI, HIDEHIRO ONODERA, JUN-WANG TANG, JINHUA YE, TAKEHIKO MATSUMOTO, National Institute for Materials Science — MIn_2O_4 (M = alkali earth metal) semiconductors show the novel photocatalytic activity under visible light irradiation. It has been reported that the activity, K, for Methylene Blue (MB) degradation is increased with decreasing the atomic radius of M, $K(CaIn_2O_4) > K(SrIn_2O_4)$. We investigate the electronic state by using the ab initio pseudopotential calculations and reveal the meaning of the classical atomic radius in the activity. $CaIn_2O_4$ and $SrIn_2O_4$ have the similar electronic structure but the band gap of $CaIn_2O_4$ becomes larger than that of $SrIn_2O_4$. It is directly connected to the photocatalytic effect. The difference is attributed to the shape of the ionic core potential. Both compounds have the same number of valence electrons. However Ca with the smaller atomic radius has the sharper and deeper ionic core potential than Sr. As a result, the valence band shifts to the lower energy state, leading to the large band gap. The classical explanation from viewpoint of atomic size is resulting in the argument of the shape of the ionic core potential. It is also found that the atomic distortion is more pronounced in $CaIn_2O_4$. The effect of the atomic distortion is also discussed.

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