Abstract Submitted
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Studies of the electronic structures of tantalum oxynitride perovskites, ATaO$_2$N (A = Ca, Sr, Ba) and PrTaON$_2$ SPENCER PORTER, Ohio State University, Chemistry, YOUNG-IL KIM, Yeungnam University, PATRICK WOODWARD, Ohio State University, Chemistry — Transition metal oxynitrides are of interest for use as photocatalysts, pigments, battery electrodes, high-permittivity dielectrics, etc. The tantalum oxynitride perovskites are of particular interest because they have band gaps that fall in the visible range of the spectrum and show excellent chemical stability. For applications such as photocatalysis the absolute positions of the valence and conduction bands play an important role. The valence and conduction band positions of ATaO$_2$N (A = Ca, Sr, Ba) and RTaON$_2$ (R = La, Pr) are characterized using a combination of diffuse reflectance UV-Visible spectroscopy, density functional theory calculations, X-ray photoelectron spectroscopy and photoelectrochemical measurements. Changes in the position of the conduction band edge, resulting from changes in the width of the conduction band, are found to play the major role in changing the band gap energy. Studies of the band positions are augmented with photocatalytic measurements demonstrating the link between band positions and photocatalytic activity.

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