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Evaluation of the band-gap of Ruddlesden-Popper tantalates JUAN RAMIREZ DE ARELLANO, SABINA RUIZ CHAVARRIA, Facultad de Ciencias, PABLO DE LA MORA, Facultad de Ciencias, Universidad Naciona Autonoma de Mexico, HOOVER A. VALENCIA, Universidad Tecnológica de Pereira, Colombia, GUSTAVO TAVIZON, Facultad de Quimica, Universidad Naciona Autonoma de Mexico — Tantalum-oxide based laminar compounds are suitable systems to perform water photo splitting reactions since the gap associated to the exciton formation has advantages over other systems. In the Ruddlesden-Popper series of compounds $A'_2[A_{n-1}B_nO_{3n+1}]$, where B=Ta and A=Lanthanide, for n=2 and 3, we have studied the effect of the A= La, Nd and Pr on the gap value, and compare our results to the experimental values for those systems. We also discuss the experimental results of the water intercalated compounds in the water splitting reaction in light of our results on the electronic structure calculations. We have evaluated the band-gap of these compounds with the WIEN2k package using the modified Becke Johnson exchange potential.

Pablo de la Mora
Facultad de Ciencias

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