Abstract Submitted
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The electronic structures of Cu delafossites nanocrystals for PEC hydrogen production: A density functional theory study[1] MUHAMMAD N. HUDA, Physics Department, University of Texas at Arlington, YANFA YAN, MOWAFAK M. AL-JASSIM, National Renewable Energy Laboragory — Efficient photo-electrochemical (PEC) splitting of water to hydrogen by sun light usually requires that the semiconductor which will be used as a photoelectrodes will satisfy several electronic criteria. As naturally available semiconductors do not meet all these criteria, a thorough understanding of "band-engineering" for mixed alloys both at bulk and nano phases is necessary to successfully design these photoelectrodes. Recently Cu delafossites, CuMO$_2$, have received much attentions as photo-catalysts for hydrogen production due to their unique properties such as stability in most aqueous solutions and excellent hole mobility. However, due to their large optical band gap they can absorb sun light only in the ultra-violet region. Hence, it is necessary to tailor their electronic properties to enhance their catalytic activities in the visible light regions. In this presentation density functional study of the Cu-delafossite nanocrystals will be presented. The stability of the nanocrystals will be discussed along with the reactivity of the different crystal faces. It will be shown that O-terminated$M$-O octahedrons play a major role in the stability of these nanocrystals, which also makes these surfaces less reactive. We will discuss the charge (electron-hole) separation problems in these nanocrystals.

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