Abstract Submitted
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Electronic structure and optical properties of $CuYO_2$ nanocrystals[1] MUHAMMAD HUDA, Department of Physics, University of Texas at Arlington, YANFA YAN, Department of Physics, University of Toledo, JOHN A. TURNER, MOWAFAK M. AL-JASSIM, National Renewable Energy Laboratory, Golden, CO — A unique class of highly stabile, self-saturated and self-charge-compensated delafossite nanocrystals has been identified. The density functional theory (DFT) study of structural and electronic properties of these nano-crystalline $CuYO_2$ will be presented. To have a better estimate of the electronic excitation energies, and consequently the optical gap, time dependent DFT has been employed as well. The goal is to show, first of all, that these unique set of nanocrystals exists, and to study whether the nano-phase can modify the electronic properties for enhanced optical absorption. It has potential application as photocatalysts for H_2 production by water splitting.

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