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Electronic structure of self-passivated Cu-delafossite nanocrystals[1] MUHAMMAD N. HUDA, Department of Physics, University of Texas at Arlington, Arlington, Texas 76019 — 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 Cu-based delafossites 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 enhance the electronic properties for its application as photocatalysts.

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Muhammad N. Huda
Department of Physics, University of Texas at Arlington,
Arlington, Texas 76019

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