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New crystal structures in hexagonal $CuInS_2$ nanocrystals XIAO SHEN, EMIL A. HERNÁNDEZ-PAGAN, Vanderbilt University, WU ZHOU, Vanderbilt University and Oak Ridge National Lab, YEVGENIY S. PUZYREV, Vanderbilt University, JUAN C. IDROBO, Oak Ridge National Lab, JANET E. MACDONALD, Vanderbilt University, STEPHEN J. PENNYCOOK, Oak Ridge National Lab, SOKRATES T. PANTELIDES, Vanderbilt University and Oak Ridge National Lab — $CuInS_2$ is one of the best candidate materials for solar energy harvesting. Its nanocrystals with a hexagonal lattice structure that is different from the bulk chalcopyrite phase have been synthesized by many groups. The structure of these $CuInS_2$ nanocrystals has been previously identified as the wurtzite structure in which the copper and indium atoms randomly occupy the cation sites. Using first-principles total energy and electronic structure calculations based on density functional theory, UV-vis absorption spectroscopy, X-ray diffraction, and atomic resolution Z-contrast images obtained in an aberration-corrected scanning transmission electron microscope, we show that $CuInS_2$ nanocrystals do not form random wurtzite structure. Instead, the $CuInS_2$ nanocrystals consist of several wurtzite- related crystal structures with ordered cation sublattices, some of which are reported for the first time here. This work is supported by the NSF TN-SCORE (JEM), by NSF (WZ), by ORNL's Shared Research Equipment User Program (JCI) sponsored by DOE BES, by DOE BES Materials Sciences and Engineering Division (SJP, STP), and used resources of the National Energy Research Scientific Computing Center, supported by the DOE Office of Science under Contract No. DE-AC02-05CH11231.

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