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Recent Progress on Modeling H Passivated CdS Nanocrystals using ab initio techniques[1] CHAD JUNKERMEIER[2], JINLING ZHOU, JAMES P. LEWIS, Dept. of Physics, West Virginia University — Spherical CdS nanocrystals with shells of H atoms are studied via an *ab initio* tight-binding analysis. Starting from the bulk zinc blende structure of CdS, these nanocrystals undergo relaxation as the geometries optimize to configurations that minimize internal forces. H atoms are then attached, to passivate the surface, and then whole structure is relaxed. We will present our latest results.

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