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Intrinsic Surface States in Semiconductor Nanocrystals: HgS Quantum Dots JAMES SIMS, GARNETT BRYANT, HOWARD HUNG, NIST — Confined states in typical nanocrystals are localized to the dot interior. Surface states are extrinsic states localized at unsaturated dangling bonds or surface defects. We show that intrinsic surface states occur in nanocrystals made from negative gap semiconductors such as HgS. We use atomistic tight-binding theory which allows explicit atomic models for the surfaces. We consider spherical HgS nanocrystals with saturated dangling bonds and diameters up the bulk limit. In small HgS dots, the lowest conduction band states are cation-derived and the band-edge valence states are anion-derived, as for finite-gap dots. In bigger HgS dots, valence states and higher conduction band states evolve toward their bulk limits. However, the lowest conduction band state has high density at the surface and slowly decays into the dot. Band mixing is critical for this state. It has mixed cation and anion character and is partly s- and light-hole-like. As the dot size increases, this conduction state crosses the valence band edge, reaching a limit inside the bulk negative gap for very large dots. In this limit, the state is localized to the surface. The optical response of Hgs dots is discussed to identify signatures for intrinsic surface states.

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