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Excitons in Negative Band Gap Nanocrystals JAMES SIMS, GARNETT W. BRYANT, HOWARD HUNG, National Institute of Standards and Technology — Exploiting quantum confinement in nanocrystals made from materials with negative bulk band-gap will be critical for nanosensor applications in the far infrared. However, understanding quantum confinement, excitonic states and optical response in negative band-gap nanocrystals provides challenges not posed for usual nanocrystals with positive bulk band-gaps. We show that intrinsic surface states occur in nanocrystals made from negative gap semiconductors such as HgS. We use atomistic tight-binding theory that accounts for band mixing critical in negative-gap semiconductors but unimportant in positive-gap systems. Such band mixing makes effective mass theory inadequate for negative-gap nanocrystals. 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. However, in bigger HgS dots, the lowest conduction band state has a high density at the surface that slowly decays into the dot. 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 excitonic states and optical response of HgS dots are discussed to identify signatures for intrinsic surface states and to assess nanosensor applications with these systems.

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