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Structure and electronic properties of gold-tipped CdSe nanorods[1] ROBERT N. BARNETT, UZI LANDMAN, Georgia Institute of Technology — We investigate CdSe nanorods capped by gold contacts and passivated by phospho-organic molecules of varying chain length. The geometry is optimized and the electronic structure obtained using first-principles quantum mechanical methods. We discuss the formation of Schottky barriers, the development of interfacial dipoles, the presence and extent of gap states induced by the metallic contact and of states in the semiconductor energy gap associated with the passivant carbon chains.

[1]Computations performed at the National Center for Computational Sciences

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