

Abstract Submitted  
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**Formation and Properties of CdS-Ag<sub>2</sub>S Nanorod Superlattices<sup>1</sup>**

DENIS DEMCHENKO, RICHARD ROBINSON, BRYCE SADTLER, LIN-WANG WANG, A. PAUL ALIVISATOS, Lawrence Berkeley National Laboratory, CAN ERDONMEZ, University of California, Berkeley — The mechanism of formation of recently fabricated<sup>1</sup> ordered CdS-Ag<sub>2</sub>S nanorod superlattices is explained and their elastic and electronic properties are predicted theoretically. We show that diffusion-limited growth of Ag<sub>2</sub>S islands in CdS nanorods partially contributes to the observed ordering, but cannot account for the full extent of the ordering alone. The valence force field (VFF) model results for the nanostructure show significant repulsion between Ag<sub>2</sub>S segments due to strain created by the lattice mismatch between the two materials. This suggests that the interplay between the chemical interface energy and strain drives the spontaneous pattern formation. A first principles calculation of the energy levels in the superlattice shows a nested band alignment. The nanorod superlattice therefore corresponds electronically to a sequence of quantum wells of Ag<sub>2</sub>S separated by barriers of CdS. The minibands formed in such superlattices make them desirable for applications in the solar cells. 1. R. D. Robinson, B. Sadtler, D. O. Demchenko, C. K. Erdonmez, L.-W. Wang, and A. P. Alivisatos, *Science* **317**, 355 (2007).

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