

Abstract Submitted  
for the MAR09 Meeting of  
The American Physical Society

Sorting Category: 13.2 (C)

**Morphology of  $\text{Cu}_2\text{S}$ -CdS and  $\text{Ag}_2\text{S}$ -CdS Nanorod Heterostructures**<sup>1</sup> DENIS DEMCHENKO, Virginia Commonwealth University, BRYCE SADTLER, University of California, Berkeley, HAIMEI ZHENG, A. PAUL ALIVISATOS, LIN-WANG WANG, Lawrence Berkeley National Laboratory — A partial cation exchange has been used to synthesize  $\text{Cu}_2\text{S}$ -CdS and  $\text{Ag}_2\text{S}$ -CdS nanocrystal heterostructures, with two very different morphologies.  $\text{Cu}^+$  cation exchange takes place preferentially at the ends of CdS nanorods,  $\text{Cu}_2\text{S}$  segments grow into the nanorod from both ends.  $\text{Ag}^+$  exchange is non-selective,  $\text{Ag}_2\text{S}$  islands nucleate and grow over the entire surface of the nanorod. This leads to very different patterns, striped  $\text{Ag}_2\text{S}$ -CdS superlattice with several equidistant  $\text{Ag}_2\text{S}$  segments in a CdS nanorod, and an asymmetric  $\text{Cu}_2\text{S}$ -CdS heterostructure with  $\text{Cu}_2\text{S}$  segments at the ends of the CdS nanorod. We use first-principles calculations to obtain formation energies of the different epitaxial interfaces between  $\text{Cu}(\text{Ag})_2\text{S}$  and different facets of CdS nanorods. Comparison of chemical and elastic contributions to the interface formation energy for the  $\text{Cu}(\text{Ag})_2\text{S}$ -CdS shows that the relative stability of the interfaces determines the nucleation of  $\text{Cu}(\text{Ag})_2\text{S}$  and the resulting morphology. Furthermore, since two end facets of CdS nanorod are not crystallographically equivalent a controlled asymmetric nucleation of  $\text{Cu}_2\text{S}$  can occur.

<sup>1</sup>Supported by U.S. DOE, DE-AC02-05CH11231 and NERSC.

Prefer Oral Session  
 Prefer Poster Session

Denis Demchenko  
ddemchenko@vcu.edu  
Virginia Commonwealth University

Date submitted: 21 Nov 2008

Electronic form version 1.4