Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Optical properties of II-VI structures for solar energy utilization

JOSHUA SCHRIER, DENIS DEMCHENKO, LIN-WANG WANG, Lawrence Berkeley National Laboratory — Although II-VI semiconductor materials are abundant, stable, and have direct band gaps, the band gaps are too large for optimal photovoltaic efficiency. However, staggered band alignments of pairs of these materials, and also the formation of intermediate impurity levels in the band gap (which has been demonstrated to increase the efficiency as compared to both single-junction devices), could be utilized to improve the suitability of these materials for solar energy utilization. Previous theoretical studies of these materials are limited, due to the well-known band gap underestimation by density-functional theory. To calculate the absorption spectra, we utilize a band-corrected planewave pseudopotential approach, which gives agreements of within 0.1 eV of the bulk optical gaps values. In this talk, I will present our work on predicting the optical properties of ZnO/ZnS and ZnO/ZnTe heterostructures, nanostructures, and alloys. This work was supported by U.S. Department of Energy under Contract No.DE-AC02-05CH11231 and used the resources of the National Energy Research Scientific Computing Center.

Joshua Schrier
Lawrence Berkeley National Laboratory

Date submitted: 20 Nov 2006

Electronic form version 1.4