Alloying ZnS to Create High-Performing Transparent Conducting Material (PV-6)

A joint India-U.S. research consortium funded under the *Joint Clean Energy Research & Development Center (JCERDC)*

Scientific Achievement:

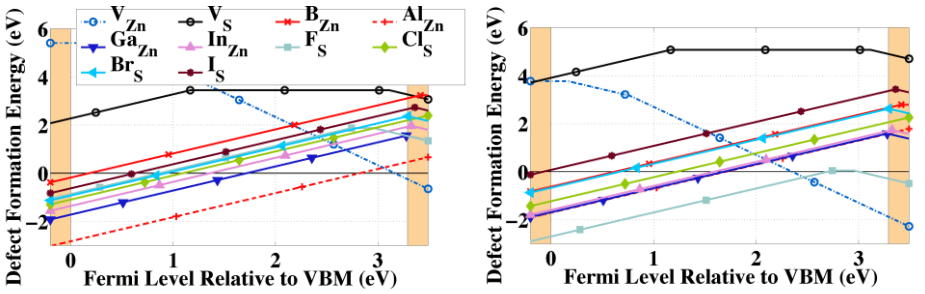
Identified the most promising n-type ZnS-based TCM as 6.25% Al-doped ZnS, with the optimal combination of physical stability, transparency, and electrical conductivity (3,830 S cm^{-1} at $n=1.0x10^{21}$ cm^{-3} and 300 K). Mobility in this material is limited by ionized impurity scattering at high carrier concentrations.

Significance and Impact:

Doped ZnS is more stable in the hexagonal structure than the cubic structure commonly synthesized. This explains the coexistence of both phases in these materials.

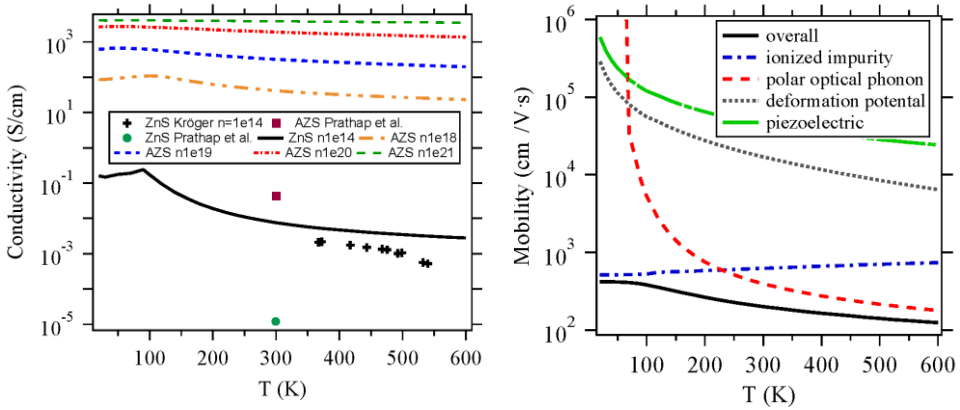
Research Details:

- Used density functional theory calculations and AMSET (*ab initio* model for mobility and Seebeck coefficient using the Boltzmann transport equation) http://www.seriius.org/modeling.html.
- Joint work with Alireza Faghaninia (WUStL Ph.D., now at LBNL) and Kunal Bhatt (IITB UG, interned at WUStL in summer 2014).



Hexagonal, Zn-rich Hexagonal, S-rich

Formation energy of defects. At each Fermi level, the most favorable charge state is plotted. The slope of the lines is equal to the charge of the defect (e.g., +1 for Al_{Zn}^{+}). We see that Al is the most soluble dopant in ZnS.



Mobility-limiting scattering mechanisms.

Publication(s): "Alloying ZnS in the Hexagonal Phase to Create High-Performing Transparent Conducting Material," *Phys. Chem. Chem. Phys.*, **18**, 22628 (2016).

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SERIIUS U.S. DEPARTMENT OF ENERGY NREL NATIONAL RENEWABLE ENERGY LABORATORY Sandia National Laboratories CSTEP RAND CORPORATION

C. Lo SERIIUS publications (peer-reviewed)

- Woods-Robinson, R. *et al.* P-Type Transparent Cu-Alloyed ZnS Deposited at Room Temperature. *Advanced Electronic Materials* (2016). doi:10.1002/aelm.201500396
- Faghaninia, A., Ager, J. W. & Lo, C. S. Ab initio electronic transport model with explicit solution to the linearized Boltzmann transport equation. *Phys. Rev. B* **91,** 235123 (2015).
- Stoica, M. & Lo, C. S. P-type zinc oxide spinels: application to transparent conductors and spintronics. *New Journal of Physics* **16,** 055011 (2014).