

Abstract Submitted  
for the CAL09 Meeting of  
The American Physical Society

**GW study of the half metallic band gap of zinc blende CrAs<sup>1</sup>**

LIAM DAMEWOOD, CHING YAO FONG, UC Davis — We determined the semiconducting gap of zinc blende (ZB) CrAs within the *GW* approximation (*GWA*). This is the first *GW* calculation of a half-metal. Previous calculations using density functional theory within the generalized gradient approximation (GGA) determined a gap of 1.8 eV, but the GGA is known to give too small of a value for this quantity in semiconductors. Additionally, since ZB CrAs is a half metal, one of its spin channels behaves like a metal and changes the quasiparticle screening compared to the insulating case. Due to the local field effect, we only included the  $\Gamma$ -point term in the metallic channel calculation of the polarizability while keeping the full set of terms in the insulating channel *GW* calculation. Preliminary results suggest these terms from the polarizability produce little change in the value of the semiconducting gap when compared to the “full” *GWA* calculation.

<sup>1</sup>This research was supported in part by the National Science Foundation Grant No. ECCS-0725902 through TeraGrid resources provided by NCSA.

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Date submitted: 16 Oct 2009

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