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GW study of the local field effect in half metallic CrAs[1] LIAM DAMEWOOD, CHING 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, we studied the role of the local field effect in CrAs. Due to the simultaneous metallic and insulating properties of half metals, the screening in CrAs is weaker compared to insulating screening. Preliminary results suggest that half metallic screening increases the semiconducting gap as much as 0.54 eV from the fully insulating value of 1.92 eV.

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