

Abstract Submitted  
for the MAR07 Meeting of  
The American Physical Society

**Effects of semicore d-electrons in screened-exchange density functional methods** BYOUNGHAK LEE, LIN-WANG WANG, Lawrence Berkeley National Laboratory — We report a theoretical study on the role of shallow  $d$  states in the screened-exchange local density approximation (sX-LDA) band structure of binary semiconductor systems. We found that the inaccurate pseudo-wavefunctions can lead to 1) an overestimation of the screened-exchange interaction between the localized  $d$  states and the delocalized higher energy  $s$  and  $p$  states and 2) an underestimation of the screened-exchange interaction between the  $d$  states. The resulting sX-LDA band structures have substantially smaller band gaps compared with experiments. We correct the pseudo-wavefunctions of  $d$  states by including the  $s$  and  $p$  states of the same shell in the valence states. The correction of pseudo-wavefunctions yields band gaps and the  $d$  state binding energy in good agreement with experiments. Compared with the quasi-particle GW method, our sX-LDA results shows not only similar quality band gaps but also much better  $d$  state binding energy. As an example, we present sX-LDA results of  $s - d$  coupling in zinc-blende semiconductors and compare them with LDA+U results. We also present an efficient method to correct the pseudo-wavefunction exchange-integral error by using projection of wavefunctions onto atomic orbitals.

Byounggak Lee  
Lawrence Berkeley National Laboratory

Date submitted: 20 Nov 2006

Electronic form version 1.4