Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

**Origin of the variation of exciton binding energy in semiconductors** MARC DVORAK, ZHIGANG WU, Colorado School of Mines — Electron-hole interaction plays a crucial role in optical properties, and the exciton binding energy ($E_b$) in technologically important semiconductors varies from merely a few meV to around 100 meV, which is not well understood. In this work, we investigate the origin of the variation of $E_b$ in semiconductors, employing first-principle calculations based on the density functional theory (DFT) and the many-body perturbation theory with Green's function (GW/BSE). Our results clearly show that $E_b$ decreases as the spread of electron distribution, which measures the magnitude of electron delocalization, increases. This is due to the increased electronic screening when electrons tend to be more delocalized. Furthermore, the spread distribution of the top valence electrons is of central importance in determining excitonic screening, which leads to weakly bound electrons and holes in semiconductors. Thus, the variation of exciton binding energy in semiconductors can be understood from the computed magnitude of electron delocalization of top valence bands of these materials using DFT.

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Date submitted: 11 Nov 2011 Electronic form version 1.4