

Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Alloy Stabilized Wurtzite Ground State Structures of Zinc-Blende Semiconducting Compounds HONGJUN XIANG, SUHUAI WEI, National Renewable Energy Laboratory, SHIYOU CHEN, XINGAO GONG, Surface Science Laboratory and Department of Physics, Fudan University, China — Although the ground state structures of zinc-blende (ZB) alloys have been extensively studied, the knowledge of the ground state structures of wurtzite (WZ) alloys remains incomplete. Here, the ground state structures of the $A_xB_{1-x}C$ WZ alloys with $x=0.25, 0.5, \text{ and } 0.75$ are revealed by a ground state search using the valence-force field model and density-functional theory total energy calculations. It is shown that the ground state WZ alloy always has a lower strain energy and formation enthalpy than the corresponding ZB alloy. Therefore, we propose that the WZ phase can be stabilized through alloying. This novel idea is supported by the fact that the WZ $AlP_{0.5}Sb_{0.5}$, $AlP_{0.75}Sb_{0.25}$, $ZnS_{0.5}Te_{0.5}$, and $ZnS_{0.75}Te_{0.25}$ alloys in the lowest energy structures are more stable than the corresponding ZB alloys. To our best knowledge, this is the first example where the alloy adopts a structure distinct from both parent phases.

Hongjun Xiang
National Renewable Energy Laboratory

Date submitted: 18 Nov 2008

Electronic form version 1.4