Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Γ-phonons in $ZnSe(C_2H_8N_2)_{1/2}$ and $ZnTe(C_2H_8N_2)_{1/2}$ hybrid materials IVAN NAUMOV, HUAXIANG FU, Department of Physics, University of Arkansas — Artificially synthesized organic/inorganic hybrid materials with semiconductor component are of growing interest due to potential applications in flexible microelectronics. Among them, hybrid $ZnSe(C_2H_8N_2)_{1/2}$ and $ZnTe(C_2H_8N_2)_{1/2}$ are two examples capable of tuning electronic and optical properties on a wide range. Engineering of these materials is difficult without deeper understanding of their fundamental physical characteristics, including electronic band structure and phonon spectra. Recent experimental investigations [1] performed on β–$ZnTe(C_2H_8N_2)_{1/2}$ samples and showed multiple sharp phonon modes in frequencies very different from the LO(Γ) phonon of the binary semiconductor ZnTe. Motivated by these results, we have performed density-functional calculations of the Γ phonon modes for both α– and β–phases of $ZnSe(C_2H_8N_2)_{1/2}$ and $ZnTe(C_2H_8N_2)_{1/2}$. We found, in particular, that light hydrogen atoms not only define the high frequency motion (1500–3000 cm^{-1}), but also dominate in some low frequency modes in the region of 100–150 cm^{-1} where they move mostly perpendicular to the superlattice stacking direction. Based on symmetry of the materials, the Raman modes at the Γ point are identified.
[1] X. Huang, J. Li, Y. Zhang, and A. Mascarenhas, J. Am. Chem. Soc. **125**, 7049 (2003).

Ivan Naumov
Department of Physics, University of Arkansas

Date submitted: 13 Nov 2006 Electronic form version 1.4