Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Mechanical and electronic properties of organicinorganic hybrid semiconductor ZnSe(C2H8N2)1/2 AMJAD NAZZAL, HUAXIANG FU, Department of Physics, University of Arkansas, Fayetteville, Arkansas 72701 — Organic–inorganic semiconductor, $ZnSe(C_2H_8N_2)_{1/2}$, under hydrostatic pressure is studied by using a first-principles pseudopotential method with mixed-basis set[1], aiming to understand its mechanical and electronic properties. With respect to the parental inorganic bulk, the hybrid is found to be nearly as twice as flexible, with a bulk modulus smaller than most known semiconductor bulks. Our calculations also demonstrate that the pressure dependence of the band gap in the hybrid semiconductor shows much pronounced nonlinearity than in bulk ZnSe. Further, our results reveal an interesting pressure-induced isoelectronic phase transition by which the in-plane hole mobility along a given direction can be drastically varied. (This work was supported by NSF-MRSEC). [1] H. Fu and O. Gulseren, PRB 66 (02) 214114.

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Date submitted: 06 Dec 2004 Electronic form version 1.4