Abstract Submitted for the MAR08 Meeting of The American Physical Society

Direct bandgap of group IV semiconductors by uni-axial stress FENG ZHANG, Department of Physics, Penn State University, PEIHONG ZHANG, Department of Physics, SUNY at Buffalo, VINCENT CRESPI — We theoretically examine the possibility of converting typical group IV semiconductors Si, SiGe (zinc blende), and Ge into direct bandgap materials by uniaxial stress along the <111>and <100> directions. For silicon, the required tensile strain is too large to be practical. For SiGe and Ge along <111>, although band splitting at the L point lowers the conduction band edge at L, a direct bandgap can still be achieved through a supralinear decrease in the energy of the conduction band edge at Γ . The required longitudinal strains along <111> are 8% and 4% for GeSi and Ge, respectively. For strain along <100>, the position of the conduction band edge at the Γ point varies sub-linearly with strain; therefore strain along $\langle 100 \rangle$ is less efficient: GeSi is unlikely to achieve a direct gap by extension along <100> and Ge requires a 6% longitudinal strain. The full dependence of the indirect/direct transition on arbitrary combinations of uniaxial/hydrostatic tensile strain is given for both GeSi and Ge.

> Feng Zhang Department of Physics, Penn State University

Date submitted: 05 Dec 2007

Electronic form version 1.4