## Abstract Submitted for the MAR15 Meeting of The American Physical Society

Band Structure and Optical Properties of Dilute Ge:C Alloys CHAD STEPHENSON, WILLIAM O'BRIEN, MENG QI, Department of Electrical Engineering, University of Notre Dame, MICHAEL PENNINGER, WILLIAM SCHNEIDER, Department of Chemical and Biomolecular Engineering, University of Notre Dame, MIRIAM GILLETT-KUNNATH, JAROSLAV ZAJICEK, Department of Chemistry and Biochemistry, University of Notre Dame, MARK WISTEY, Department of Electrical Engineering, University of Notre Dame — The last major missing piece to achieving integrated Si photonics is an efficient light emitter. Dilute Ge:C alloys offer a new route to create efficient lasers directly within conventional CMOS electronics. Although neither Ge nor C emits light, Ge:C is a highly mismatched alloy, similar to GaAsN, in which band anticrossing is expected to create a direct bandgap. We have performed ab initio band structure simulations using hybrid functionals and spin-orbit coupling that show a sharp decrease in bandgap at the direct conduction band valley with C incorporation, turning Ge:C into a direct bandgap semiconductor and even a semi-metal. We report on the optical properties, highlighting the strength of free carrier absorption due to the changes in the band structure. Some of its potential applications include integrated light emitters, modulators, and photodetectors. With the three-band system, Ge:C also has potential for use in upconverting structures. We also report successful incorporation of C in Ge using hybrid gas+solid source molecular beam epitaxy (MBE) using a precursor gas, tetra(germyl)methane (4GeMe), that prevents undesirable C-C bonds and interstitial incorporation.

> Chad Stephenson University of Notre Dame

Date submitted: 14 Nov 2014

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