Abstract Submitted for the MAR07 Meeting of The American Physical Society

Si-Ge Intermixing and the 5x5-(111) Surface Reconstruction<sup>1</sup> DEMETRA PSIACHOS, M. J. STOTT, Department of Physics, Queen's University — We present *ab initio* results of the energetics and structure of a Si(111)-5x5 slab with two bilayers of Ge(5x5) adsorbed on it. We explore the aspects of this Si-Ge surface structure with those of an analogous pure Ge(111)-5x5 slab and we note many important differences such as the larger corrugation of the adatom heights in the former compared with the latter. *Ab initio* results are also obtained for the effects of Si-Ge intermixing at the Si-Ge interface. These shed light on this transport mechanism as a way of lowering the strain.

<sup>1</sup>Work supported by the NSERC of Canada

Demetra Psiachos Department of Physics, Queen's University

Date submitted: 20 Nov 2006

Electronic form version 1.4