Abstract Submitted for the MAR14 Meeting of The American Physical Society

Substrate effect on the band gap of semiconducting atomic wires<sup>1</sup> ADAM J. SIMBECK, Rensselaer Polytechnic Institute, SAROJ K. NAYAK, Rensselaer Polytechnic Institute, Indian Institute of Technology Bhubaneswar — The electronic structure of free-standing and supported semiconducting atomic wires is investigated using a combination of first-principles density functional theory (DFT) and many-body perturbation theory (MBPT). The band gaps predicted from DFT for SiH<sub>2</sub> and GeH<sub>2</sub> atomic wires are unaffected by the presence of the substrate, whereas the gaps calculated using MBPT under the GW approximation are reduced by about 1eV when the wires are supported. The reduction in the band gap is attributed to a change in the electronic correlation energy, which can be understood as a screened Coulomb interaction. These results highlight the importance of the role played by the substrate in manipulating the electronic and optical properties of quantum confined Si and Ge systems.

<sup>1</sup>Work supported by the Interconnect Focus Center (MARCO program), State of New York, NSF IGERT Program, Grant no. 0333314, NSF Petascale Simulations and Analysis (PetaApps) program, Grant No. 0749140, and computing resources of the CCNI at RPI.

Adam Simbeck Rensselaer Polytechnic Institute

Date submitted: 14 Nov 2013

Electronic form version 1.4