Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Universal behavior of surface-dangling bonds in hydrogen-terminated Si, Ge, and Si/Ge nanowires.[1] RICARDO NUNES, Universidade Federal de Minas Gerais - UFMG, RICARDO KAGIMURA, HÉLIO CHACHAM, UFMG — We report an *ab initio* study of the electronic properties of surface dangling bond (SDB) states in hydrogen-terminated Si, Ge, and Si/Ge nanowires with diameters between 1 and 2 nm. We find that the charge transition levels $\varepsilon(+/-)$ of SDB states are deep in the bandgap for Si wires, and shallow (near the valence band edge) for Ge wires. In both Si and Ge wires, the SDB states are localized. We also find that the SDB $\varepsilon(+/-)$ levels behave as a "universal" energy reference level among Si, Ge, and Si/Ge wires within a precision of 0.1 eV. By computing the average bewteen the electron affinity and ionization energy in the atomi limit of several atoms from the III, IV and V columns, we conjecture that the universality is a periodic-table atomic property.

[1]Acknowledge support from CNPq, FAPEMIG, and Instituto do Milênio de Nanotecnologia - MCT/Brazil

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Date submitted: 05 Dec 2006 Electronic form version 1.4