Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

First-principle calculations of molecular conductance with semiconducting electrodes NORIHIRO ITO, HISAO NAKAMURA, KOICHI YAMASHITA, The University of Tokyo — For molecular electronics, many researches have been performed about molecular conductance with gold electrodes. However, several recent experiments have demonstrated the feasibility of attaching various molecules on silicon surfaces. So, we study molecular junction formed on silicon surface. We calculate conductance of systems included pure silicon and phosphorus-doped silicon electrodes. In order to calculate the conductance, we adopt nonequilibrium Green's function theory combined with density functional theory (NEGF-DFT). We consider several molecules and atomic wires sandwiched between pure Si (100) electrodes or P-doped Si (100) electrodes. In our DFT calculation, the band gap value of the pure bulk silicon is about 0.554 eV. In our model, phosphorus-doped silicon electrodes are composed of P/Si in the ratio 1: 63 and the resulting doped electrodes show the metallic features. In the case of pure silicon electrodes transmission coefficients are about equal to zero in the energy ranges of $E_F \pm 0.38$ eV, while in the case of phosphorus-doped silicon electrodes transmission coefficients take finites values.

Norihiro Ito
The University of Tokyo

Date submitted: 23 Nov 2007 Electronic form version 1.4