Abstract Submitted
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Transport Properties of Nanoscale Materials by First-principles Calculations HIROSHI MIZUSEKI, RODION V. BELOSLUDOV, S.-U. LEE, YOSHIYUKI KAWAZOE, Institute for Materials Research, Tohoku Univerisity — Molecular devices are potential candidates for the next step towards nanoelectronic technology. Our group has covered a wide range of nanoscale wires, which have potential application in molecular electronics using first-principles calculations and nonequilibrium Green's function formalism [1]. Our target materials are supramolecular enamel wires (covered wires) [2], connection between organic molecules and metal electrodes, self-assembled nanowires on silicon surface [3], porphyrin [4], phthalocyanine, metallocene [5], fused-ring thiophene molecules, length dependence of conductance in alkanedithiols and so on. Namely, we have investigated a relationship of the energy levels of delocalized frontier orbitals (HOMO and LUMO) and Fermi level of metal electrodes and estimate the electronic transport properties through atomic and molecular wires using Green's function approach. References [1] http://www-lab.imr.edu/∼mizuseki/nanowire.html [2] R. V. Belosludov, A. A. Farajian, H. Baba, H. Mizuseki, and Y. Kawazoe, Jpn. J. Appl. Phys., **44**, 2823 (2005). [3] R. V. Belosludov, A. A. Farajian, H. Mizuseki, K. Miki, and Y. Kawazoe, Phys. Rev. B, **75**, 113411 (2007). [4] S.-U. Lee, R. V. Belosludov, H. Mizuseki, and Y. Kawazoe, Small **4** (2008) 962. [5] S.-U Lee, R. V. Belosludov, H. Mizuseki, and Y. Kawazoe, J. Phys. Chem. C. **111** (2007) 15397.

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