Abstract Submitted
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Transport Properties through Nanomaterials by First-principles Calculations HIROSHI MIZUSEKI, RODION BELOSLUDOV, SANG UCK LEE, YOSHIYUKI KAWAZOE, Institute for Materials Research, Tohoku University, IMR TEAM — Nanoscale molecular devices are potential candidates for this next step, and they would make it possible to realize the most advantageous devices. Our group has covered a wide range of nanoscale materials[1] such as self-assembled nanowires on Si(001) [2, 3], quantum length dependence of conductance in oligomers [4] and single-molecule rotation switch [5] and so on. In this presentation, we will present our recent study on the transport properties of these nanoscale materials using the nonequilibrium Green's function formalism for quantum transport and the density functional theory (DFT) of electronic structures using local orbital basis sets. References 1. http://www-lab.imr.edu/∼mizuseki/nanowire.html 2. J.-T. Wang, C. Chen, E. G. Wang, D.-S. Wang, H. Mizuseki, and Y. Kawazoe, Phys. Rev. Lett., 97 (2006) 046103. 3. R. V. Belosludov, A. A. Farajian, H. Mizuseki, K. Miki, and Y. Kawazoe, Phys. Rev. B, 75 (2007) 113411. 4. Y. X. Zhou, F. Jiang, H. Chen, R. Note, H. Mizuseki, and Y. Kawazoe, Phys. Rev. B, 75 (2007) 245407. 5. Y. Y. Liang, F. Jiang, Y. X. Zhou, H. Chen, R. Note, H. Mizuseki, and Y. Kawazoe, J. Chem. Phys. 127 (2007) 084107.

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