Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Electronic Structure of Aromatic and Quinoidic Oligothiophenes by First-principles Calculations HIROSHI MIZUSEKI, YOSHIYUKI KAWAZOE, Institute for Materials Research, Tohoku Univerisity — Since the discovery in 1977 that trans-polyacetylene can be made electrically conducting by means of doping[1] several different conjugated polymers with interesting properties in the conducting and semiconducting phases have been discovered. Polythiophene has a typical π-conjugated system, then many polythiophenes are synthesized and several have been well characterized. Calculation systems based on neutral, doubly charged, and highly charged oligomers whose all ring are linked to have linear chains were studied as model for the polaronic defects in doped polythiophenes. The energetics of the aromatic and quinoid structures is investigated using the both ends of neutral oligomers substituted by dimethyl and dimethylen. To estimate the electronic structures, the difference between corresponding bond lengths along the C-C path of neutral, dicationic, and dianionic oligomers, were investigated. Calculations were performed on systems containing 16 monomers, by using B3LYP/6-31G(d) level of theory. References [1] C. K. Chiang et al., Phys. Rev. Lett. 39, 1098 (1977). [2] http://www-lab.imr.edu/∼mizuseki/nanowire.html

Hiroshi Mizuseki
Institute for Materials Research, Tohoku Univerisity

Date submitted: 20 Nov 2008 Electronic form version 1.4