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***Ab* initio study of solvent effects on electrical transport of molecular bridge between electrodes** ARIHIRO TAWARA, TOMOFUMI TADA, SATOSHI WATANABE, Department of Materials Engineering, Graduate School of Engineering, The University of Tokyo and CREST, Japan Science and Technology Agency — The electrical conductance of benzene dithiolate (BDT) between gold electrodes has been actively investigated to realize single molecular devices. However, almost all of previous theoretical studies for the electrical conductance of BDT were done assuming 0K and vacuum in spite that many measurements have been performed at room temperature in solution [1,2]. In this study, we have investigated the electrical transport of BDT molecule between gold electrodes in water solution using *ab initio* nonequilibrium Green's function method and Car-Parrinello molecular dynamics at room temperature. The calculated time-averaged conductance of the BDT in water solution, 0.190 G_0, is clearly different from the value calculated without water, 0.201 G_0. Detailed analysis shows that this difference can be attributed to the effect of dipole moments of water molecules on the potential profile of the BDT molecule. [1] X. Xiao *et al.*, Nano Lett. **4**, 267 (2004). [2] M. Kiguchi *et al.*, Appl. Phys. Lett. **89**, 213104 (2006).

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