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Ab initio Green's function method and Boltzmann averaging for electrical conductance of a single molecular junction TOMOFUMI TADA, ARIHIRO TAWARA, TOSHIYA MATSUYAMA, SATOSHI WATANABE, Department of Materials Engineering, The University of Tokyo, CREST-JST, SATORU TANIBAYASHI, HIDEO SEKINO, Department of Knowledge-Based Information Engineering, Toyohashi University of Technology — The electrical conductance through benzene-dithiolate (BDT) between gold electrodes is studied using ab initio Green's function method coupled with GAUSSIAN 03 [1]. To simulate break junction experiments of BDT [2], we consider the energetic stability of transient structures of the BDT junction and possibility of the fluctuation among several structures, because these points have not been examined yet in spite that they may affect measurements results considerably. For this purpose, the most probable conductance of BDT is estimated by taking an average using Boltzmann factor [3]. The averaged conductance shows good agreement with the observed conductance and also shows a flat plateau just before the break of the junction, which is also observed by Xiao et al. [2]. We further investigate solvent effects on conductance by including solvent molecules between electrodes. The results for solvent effects will be presented at the meeting. [1] T. Tada et al., J. Chem. Phys. 121, 8050 (2004). [2] Xiao et al., Nano Lett. 4, 267 (2003). [3] S. Tanibayashi et al., Chem. Phys. Lett. 428, 367 (2006).

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