

Abstract Submitted  
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**The current-voltage characteristic of a metal-molecule-metal junction studied by an integrated and piecewise thermal equilibrium approach**<sup>1</sup> Y.-H TANG, T.-H LU, M.-H. TSAI, Department of Physics, National Sun Yat-Sen University, Kaohsiung 80424, Taiwan — The current-voltage characteristic of a metal-molecule-metal junction has been studied by a new approach. The Au electrodes are modeled by 3-layer (111) films and the self-assembled monolayer (SAM) of Au-benzene-1,4-dithiol-molecule-Au molecules is sandwiched between them. The non-equilibrium electron distribution function is approximated by the Fermi-Dirac distribution function with a position dependent chemical potential to reflect spatial variation of the local electrostatic potential. The electronic states of the whole Au-film-SAM-Au-film system are calculated and are regarded as standing waves, which can be decomposed into  $+z$  and  $-z$  moving waves,  $\Psi_+$  and  $\Psi_-$ , respectively, where  $z$  is the coordinate normal to the films. The current per molecule is obtained from the standard quantum mechanical current densities of the  $\Psi_+$  and  $\Psi_-$  states. With this approach the calculated I-V characteristic is improved substantially with respect to those obtained by the conventional transmission-probability-Green-function type approaches..

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