Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Electronic structures of self-assembled monolayer of molecules of symmetric disulfides of benzoic acid[1] Y. -H. TANG, M. -H. TSAI, National Sun Yat-Sen University, Kaohsiung 804 Taiwan — Electronic structures of self-assembled monolayer (SAM) of molecules of symmetric disulfides of benzoic acid have been studied using the first-principles calculation method. The functional elements considered are H, Br and F. It is found that the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) are composed mainly of S orbital at the end and C-H bonding orbitals in the middle benzene-ring of the molecule, respectively. The separation between HOMO and LUMO energy levels (bands) are found to be less than 1.0eV. It is also found that when the distance between adjacent molecules are small enough, SAM becomes semimetallic due to lateral couplings among molecules. The dipole moments per molecule of these SAM's with Br and F functional elements are found to decrease substantially when the lateral distance between molecules is reduced. The electronic structure of SAM or a single organic molecule used for molecular electronics is often treated as unaltered under an applied electric field in the calculation of electric current using the Green function method. However, an applied field is found to cause significant redistribution of charges in the molecule.

[1]Supported by National Center for Theoretical Sciences (South) of ROC.

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Date submitted: 30 Nov 2004 Electronic form version 1.4