Surface properties of substituted-benzenethiol monolayers on gold and silver: Work function, wettability and surface tension

Shingo Tatara¹, Yasutaka Kuzumoto², and Masatoshi Kitamura¹,³*

¹Department of Electrical and Electronic Engineering, Graduate School of Engineering, Kobe University, Kobe 657-8501, Japan
²Advanced Technology Research Laboratories, Sharp Corporation, Tenri, Nara 632-8567, Japan
³Institute for Nano Quantum Information Electronics (NanoQuine), The University of Tokyo, Meguro, Tokyo 153-8505, Japan
*E-mail: kitamura@eedept.kobe-u.ac.jp

Supplementary Information

1. Mulliken charges

Figure S1 shows the Mulliken charges calculated for molecules with chemical structures shown in this figure. The value of the Mulliken charge was obtained using the Gaussian 09 software package. The charge of a hydrogen atom is summed into the charge into the heavy atom with which the hydrogen atom bounds.

![Mulliken charges](image)

Fig. S1. Mulliken charges calculated for a molecule with a S-Au or S-Ag group instead of a S-H group in MBT, BT, FBT, or PFBT.
2. Water contact angles

Figure S2 shows water contact angles measured on Au surfaces modified with various substituted BTs and unmodified. The substituted BT on the horizontal axis is placed in the decreasing order in water contact angle. The plot is shown as visual description of difference in water contact angle among the substituted BTs. Although the horizontal axis does not have physical meaning at this point, a physical factor for the order may be found from theoretical investigation.

![Fig. S2. Water contact angles on Au surfaces modified with various substituted BTs and unmodified.](image)

3. Surface tensions

Figure S3 shows the surface tension $\gamma_s$, the dispersion component $\gamma_s^d$, and the polar component $\gamma_s^p$ of Au surfaces modified with various substituted BTs. The substituted BT is placed in the increasing order in polar component. Thus, physical meaning for the order is unclear at this point as well as Fig. S2.

![Fig. S3. Surface tension $\gamma_s$, dispersion component $\gamma_s^d$, and polar component $\gamma_s^p$ of Au surfaces modified with various substituted BTs.](image)