Supplemental Informations

Molecular Evidence for the Intermolecular S···S Interaction in the Surface Molecular Packing Motifs of a Fused Thiophene Derivative

Xuan-Yun Wang,[a, b] Wei Jiang,[a, b] Ting Chen,[a] Hui-Juan Yan,[a] Zhao-Hui Wang,[a] Dong Wang,*[a] and Li-Jun Wan[a]

[a] *Institute of Chemistry, The Chinese Academy of Sciences, Beijing National Laboratory for Molecular Sciences, Beijing 100190, People's Republic of China. Fax & Tel: 86-10-82616935; E-mail: wangd@iccas.ac.cn*

[b] *The Chinese Academy of Sciences University, Beijing, People's Republic of China.*

Experimental Section

Trans-1,2-(dithieno[2,3-b:3′,2′-d]thiophene)ethene derivative (TDT) was synthesized according to the previous report [S1]. TDT solution was prepared using 1-phenyloctane (Acros Organics, HPLC grade) as a solvent with a concentration between 10^{-4} and 10^{-5} M. A droplet of this solution (2 μL) was deposited on a freshly cleaved atomically flat surface of HOPG (quality ZYB, Digital Instruments, Santa Barbara, CA). STM measurement was performed at the 1-phenyloctane/ HOPG interface using a Nanoscope III-SPM scanning tunneling microscope (Digital Instuments, Santa Barbara, CA) at room temperature. Mechanically cut Pt/Ir wires (90/10) were used as STM tips. The annealing experiment was carried out by heating the samples at designated temperature and then cooling down to room temperature for STM imaging. All the images were collected with the constant current mode and shown without further processing. The specific tunneling conditions are given in the corresponding figure caption. Mass spectroscopy (MS) of the sample was characterized using Waters GCT mass spectrometer. MS (EI) 584.2.

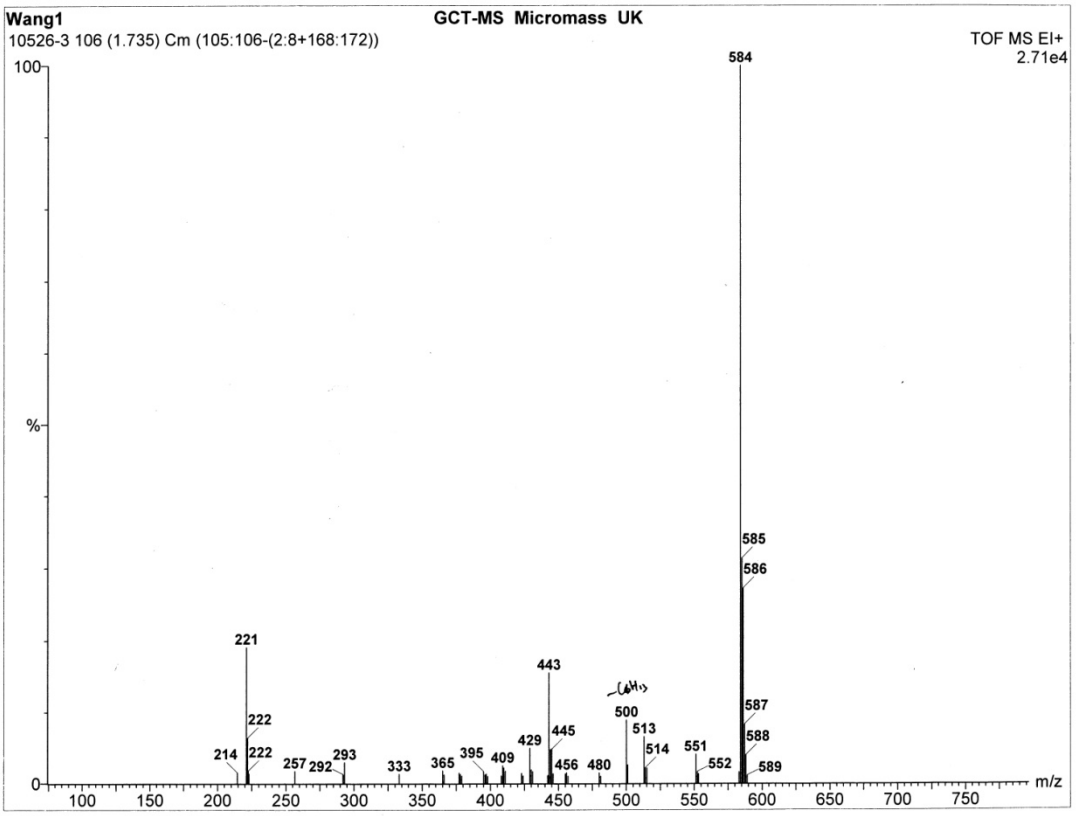

Figure S1 MS spectrogram of TDT after heating at 100 ºC for 10 min.

S1. Zhang L, Tan L, Wang Z.H., Hu W.P., Zhu D.B. High-performance, stable organic field-effect transistors based on *trans*- 1,2-(dithieno[2,3-b:3′,2′-d]thiophene) ethene. Chem. Mater. 2009, 21, 1993-1999.