Supporting Information

# Improving the thermoelectric properties of 2,7-dioctyl[1]benzothieno[3,2-b][1]benzothiophene-based organic semiconductors by isotropic strain

Ziman Wang[#,1,2], Ming Yang[#,1,2], Qinglong Jiang[3], Kun Zheng[4], Yongmei Ma[4], Hang Zhang[1,2,*]

[1]*Institute of Engineering Thermophysics, Chinese Academy of Sciences, Beijing 100190, China*
[2]*University of Chinese Academy of Sciences, Beijing 100049, China*
[3]*Department of Chemistry and Physics, University of Arkansas, Pine Bluff, Arkansas 71601, USA.*
[4]*Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China*

[#] *These authors contributed equally to this work.*
** **E-mail**: zhanghang@iet.cn*

To study the uniaxial thermoelectric parameters, we set the thermoelectric parameters in plane is the value along *a* axis and the thermoelectric parameters out plane is the average value along *b* axis and *c* axis. We provided the uniaxial thermoelectric parameters of $C_8$-BTBT-based organic semiconductor in Fig. S1. It can be seen that the in-plane values dominate both the electrical conductivity and thermal conductivity.

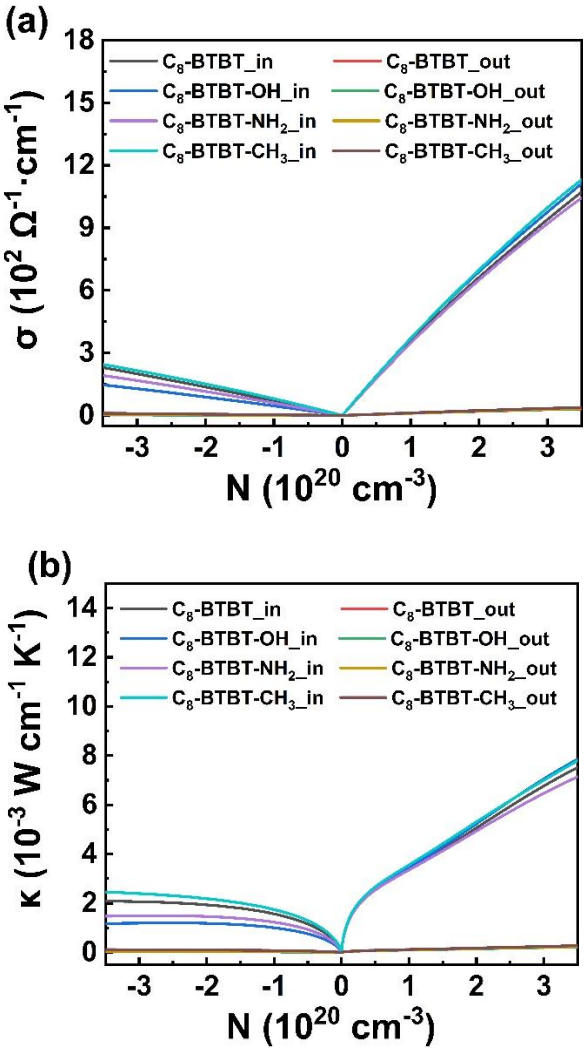
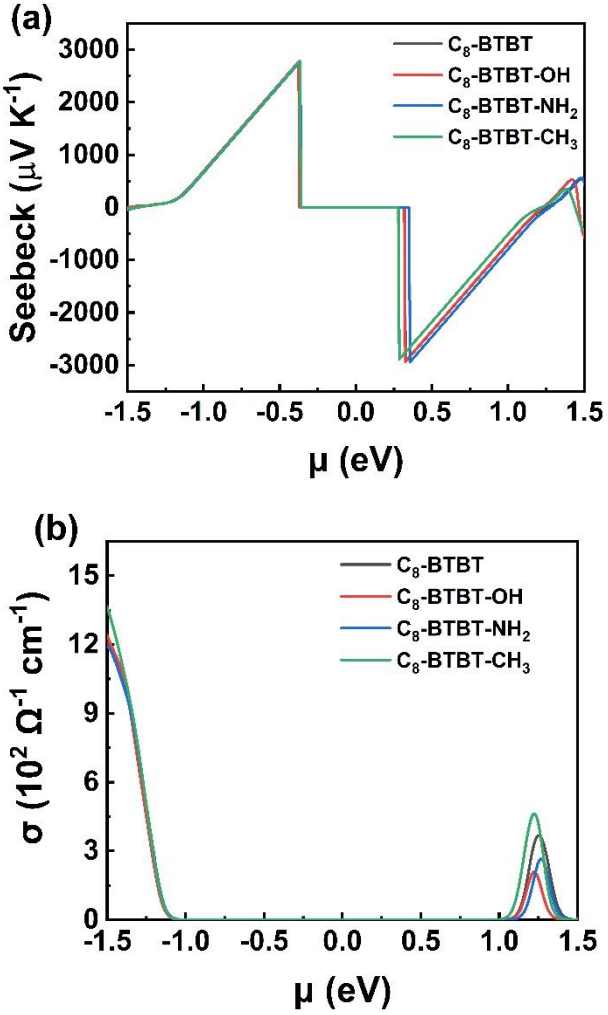



**Fig. S1** (a) Electrical conductivity, (b) thermal conductivity in plane and out plane as a function of the carrier concentration at 300K of $C_8$-BTBT-based organic semiconductor.

Fig. S2(a)-(d) represent the thermoelectric parameters of semiconductors as a function of chemical potential at 300 K. We can observe that the thermoelectric

parameters exhibit the same critical points of the chemical potential in p-type and n-type region between − 1 to + 1 eV. Following Fig. S2(a), it can be found that *S* show one peak for p-type semiconductor and one valley for n-type semiconductor at the vicinity of Fermi levels, which is also consistent with Hall coefficient ($R_H$) (Fig. S2(e)). In all cases the peak value of *S* is about 2700 μV/K while the valley value is about − 3000 μV/K. As show in Fig. S2(c), these semiconductors exhibit the minimum value of thermal conductivity at the chemical potential ranges between ±1 eV. And in Fig. S2(d), the *zT* beyond ±1 eV exhibit very sharp rise.



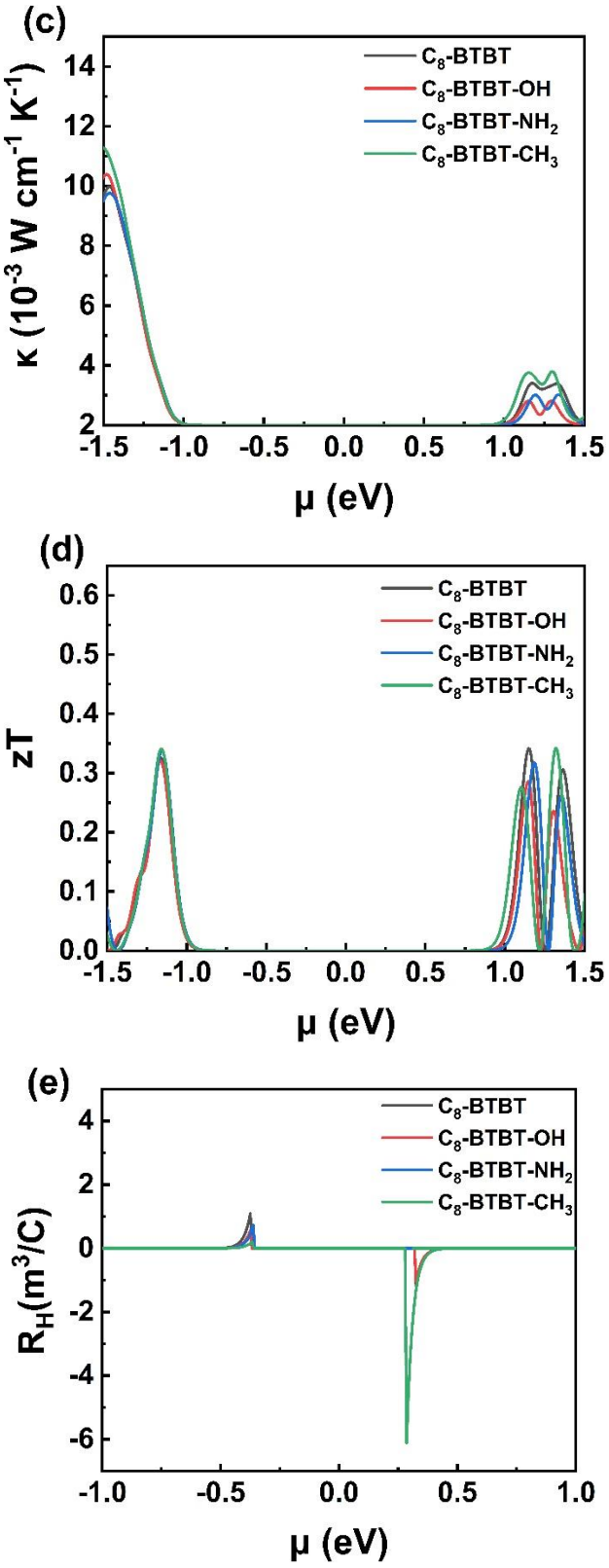



**Fig. S2** (a) Seebeck coefficient, (b) electrical conductivity, (c) thermal conductivity, (d) figure of merit and (e) hall coefficient as a function of chemical potential at 300K of $C_8$-BTBT-based organic semiconductor.