Synthesis of Siprodithienogermoles with Triphenylamine Units as a Dopant-Free Hole-Transporting Material of Perovskite Solar Cells

Joji Ohshita,^{a,b,*} Keisuke Kondo,^a Yohei Adachi,^a Myungkwan Song,^{d,*} Sung-Ho Jin^{c,*}

^a Department of Applied Chemistry, Graduate School of Advanced Science and Engineering, Hiroshima University, Higashi-Hiroshima 739-8527, Japan

^b Materials Model-Based Research Division, Digital Monozukuri (Manufacturing) Education and Research Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

^c Department of Chemistry Education, Graduate Department of Chemical Materials, Institute for Plastic Information and Energy Materials, Pusan National University, Busandaehakro 63-2, Busan 46241, Republic of Korea

^d Materials Center for Energy Convergence, Surface Technology Division, Korea, Institute of Materials Science (KIMS), 797 Changwondaero, Sungsan-Gu, Changwon, Gyeongnam 642-831, Republic of Korea

Supporting Information

- Figure S1. ¹H and ¹³C NMR spectra of sDTG-tpa in CDCl₃.
- Figure S2. ¹H and ¹³C NMR spectra of sDTG-dmap in CDCl₃.
- Figure S3. ¹H and ¹³C NMR spectra of sDTG-mop in CDCl₃.
- Figure S4. ¹H and ¹³C NMR spectra of m1 in CDCl₃.
- Figure S5. ¹H and ¹³C NMR spectra of m2 in acetone-d₆ and CDCl₃, respectively.
- Figure S6. Cyclic voltammograms (CVs) of sDTG-tpa, sDTG-dmap, sDTG-mop, m1, and m2.
- Figure S7. HOMO and LUMO profiles of sDTG-tpa, derived from DFT calculations at B3LYP/6-31G(d,p).



Figure S1. ¹H (top) and ¹³C NMR spectra (bottom) of **sDTG-tpa** in CDCl₃. An asterisk in the expanded ¹H NMR spectrum indicates an unidentified signal.



Figure S2. ¹H (top) and ¹³C NMR spectra (bottom) of **sDTG-dmap** in CDCl₃. Asterisks in the expanded ¹H NMR spectrum indicate unidentified signals.



Figure S3. ¹H (top) and ¹³C NMR spectra (bottom) of **sDTG-mop** in CDCl₃. Asterisks in the expanded ¹H NMR spectrum indicate unidentified signals.



Figure S4. ¹H (top) and ¹³C NMR spectra (bottom) of **m1** in CDCl₃. Asterisks in the expanded ¹H NMR spectrum indicate unidentified signals.



Figure S5. ¹H (top) and ¹³C NMR spectra (bottom) of **m2** in acetone-d₆ and CDCl₃, respectively. Asterisks in the expanded ¹H NMR spectrum indicate unidentified signals.



Figure S6. Cyclic voltammograms (CVs) of sDTG-tpa, sDTG-dmap, sDTG-mop, m1, and m2.



Figure S7. HOMO (left) and LUMO (right) profiles of **sDTG-tpa**, derived from DFT calculations at B3LYP/6-31G(d,p).