

Supplementary Information

Charge Carrier Formation following Energy Gap Law in Photo-Activated Organic Materials for Efficient Solar Cells

Aniket Rana ^{1,2,*,†}, Nikita Vashistha ^{2,3,†}, Amit Kumar ^{2,4†}, Mahesh Kumar ^{2,5*} and Rajiv K. Singh ^{2,4,*}

¹ Department of Chemistry and Centre for Processable Electronics, Imperial College London, London W12 0BZ, UK

² Academy of Scientific and Innovative Research (AcSIR), CSIR-NPL Campus, New Delhi 110012, India; nikita.vashistha@uni-jena.de (N.V.); kumaramitiitg004@gmail.com (A.K.)

³ Institute of Physical Chemistry, Friedrich Schiller University Jena, Helmholtzweg, 4, 07743 Jena, Germany

⁴ CSIR – National Physical Laboratory, Dr. K.S. Krishnan Marg, New Delhi 110012, India

⁵ Innovation and Management Directorate Council of Scientific and Industrial Research, Anusandhan Bhawan, New Delhi 110001, India

* Correspondence: aniket.rana@imperial.ac.uk (A.R.); rajivsingh@nplindia.org (R.K.S.); mkumar@csir.res.in (M.K.)

† These authors contributed equally to this work.

Keyword: organic solar cell, carrier dynamics, energy gap law

Table S1 The lifetime of excited carriers and associated pre-exponential amplitude for $DTS(FBTTh_2)_2$ and $DTS(FBTTh_2)_2:PC[70]BM$ at different wavelength after multi-exponential fitting.

| $DTS(FBTTh_2)_2$ | | | | | | |
|---|------------|------------|------------|-------------|-------------|-------------|
| $\lambda(nm)$ | 469 | 595 | 714 | 1078 | 1195 | 1294 |
| A1 | 0.696 | -0.683 | -0.688 | 0.631 | 0.688 | 0.638 |
| $\tau_1(ps)$ | 0.982 | 1.43 | 1.54 | 3.07 | 2.57 | 2.87 |
| A2 | 0.247 | -0.237 | -0.184 | 0.327 | 0.293 | 0.359 |
| $\tau_2(ps)$ | 19.1 | 28.4 | 46.1 | 47.9 | 31.7 | 37.7 |
| A3 (offset) | 0.057 | -0.0807 | -0.128 | 0.0418 | 0.0189 | 0.0032 |
| $DTS(FBTTh_2)_2:PC[70]BM$ | | | | | | |
| $\lambda(nm)$ | 593 | 648 | 771 | 989 | 1116 | 1311 |
| A1 | -0.339 | -0.344 | 0.518 | 0.308 | 0.173 | 0.237 |
| $\tau_1(ps)$ | 6.31 | 4.05 | 1.9 | 2.69 | 3.16 | 1.94 |
| A2 | -0.311 | -0.255 | 0.354 | 0.15 | 0.253 | 0.155 |
| $\tau_2(ps)$ | 62.2 | 57.9 | 44.7 | 229 | 209 | 261 |
| A3 | -0.232 | -0.205 | 0.098 | 0.313 | 0.349 | 0.36 |
| $\tau_3(ps)$ | 1560 | 1200 | 1130 | 1980 | 2220 | 3060 |

Table S2 The lifetime of excited carriers and associated pre-exponential amplitude for $PCE10$ and $PCE10:PC[70]BM$ at different wavelength after multi-exponential fitting.

| PCE10 | | | | | | | |
|---------------------------------|------------|------------|------------|------------|------------|-------------|-------------|
| $\lambda(nm)$ | 581 | 648 | 708 | 741 | 866 | 958 | 1119 |
| A1 | -0.816 | -0.764 | -0.71 | -0.659 | 0.8 | 0.717 | 0.603 |
| $\tau_1(ps)$ | 0.392 | 0.527 | 0.771 | 0.99 | 0.458 | 0.59 | 0.908 |
| A2 | -0.153 | -0.144 | -0.144 | -0.168 | 0.12 | 0.181 | 0.242 |
| $\tau_2(ps)$ | 15.5 | 18.4 | 17.3 | 159 | 19.5 | 21.5 | 31.5 |
| A3 (offset) | -0.0307 | -0.0757 | -0.107 | 0.112 | 0.0604 | 0.0925 | 0.119 |
| PCE10:PC[70]BM | | | | | | | |
| $\lambda(nm)$ | 661 | 702 | 775 | 877 | 979 | 1072 | |
| A1 | -0.524 | -0.562 | 0.605 | 0.378 | 0.317 | 0.263 | |
| $\tau_1(ps)$ | 1.9 | 1.7 | 1.43 | 1.71 | 1.45 | 2.59 | |
| A2 | -0.19 | -0.188 | 0.329 | 0.314 | 0.28 | 0.227 | |
| $\tau_2(ps)$ | 52.7 | 55.2 | 19.3 | 38 | 44.9 | 47.3 | |
| A3 | -0.225 | -0.191 | -0.0661 | 0.226 | 0.296 | 0.392 | |
| $\tau_3(ps)$ | 867 | 910 | inf | 884 | 1040 | 979 | |

Table S3 The lifetime of excited carriers and associated pre-exponential amplitude for PCDTBT and PCDTBT:PC[70]BM at different wavelength after multi-exponential fitting.

| PCDTBT | | | | | | |
|---------------------------------|------------|------------|------------|------------|-------------|-------------|
| λ(nm) | 514 | 553 | 658 | 986 | 1143 | 1298 |
| A1 | -0.657 | -0.556 | 0.579 | 0.303 | 0.475 | 0.742 |
| τ1(ps) | 2.55 | 2.18 | 17.2 | 3.38 | 198 | 269 |
| A2 | -0.215 | -0.22 | 0.241 | 0.232 | 0.466 | 0.258 |
| τ2(ps) | 171 | 287 | 225 | 66.3 | 1640 | inf |
| A3 | -0.129 | -0.224 | 0.172 | 0.375 | -0.0592 | 0 |
| τ3(ps) | 940 | 1110 | 1120 | 1180 | inf | 0 |
| PCDTBT:PC[70]BM | | | | | | |
| λ(nm) | 552 | 582 | 708 | 914 | 1095 | |
| A1 | -0.551 | -0.521 | 0.384 | 0.293 | 0.294 | |
| τ1(ps) | 1.98 | 1.26 | 0.86 | 3.48 | 27.5 | |
| A2 | -0.276 | -0.283 | 0.232 | 0.229 | 0.437 | |
| τ2(ps) | 398 | 729 | 75.5 | 65.6 | 630 | |
| A3 | -0.173 | -0.196 | 0.384 | 0.391 | 0.257 | |
| τ3(ps) | Inf | Inf | 1600 | 1260 | 1590 | |

Table S4 The lifetime of excited carriers and associated pre-exponential amplitude for PBDTT-DPP and PBDTT-DPP:PC[70]BM at different wavelength after multi-exponential fitting.

| PBDTT-DPP | | | | | |
|---------------------------------|------------|------------|-------------|------------|-------------|
| λ(nm) | 637 | 679 | 742 | 979 | 1167 |
| A1 | -0.701 | -0.654 | -0.649 | 0.566 | 0.61 |
| τ1(ps) | 0.447 | 1.42 | 1.63 | 2.55 | 2.75 |
| A2 | -0.235 | -0.276 | -0.28 | 0.425 | 0.386 |
| τ2(ps) | 9.73 | 28.2 | 35.9 | 31 | 36.7 |
| A3 (offset) | -0.0636 | -0.0691 | -0.071 | 0.00885 | 0.00368 |
| PBDTT-DPP:PC[70]BM | | | | | |
| λ(nm) | 745 | 928 | 1147 | | |
| A1 | 0.596 | 0.631 | 0.481 | | |
| τ1(ps) | 1.14 | 1.85 | 2.05 | | |
| A2 | -0.313 | 0.269 | 0.466 | | |
| τ2(ps) | 3.66 | 31.5 | 19.4 | | |
| A3 (offset) | -0.0629 | 0.0996 | 0.053 | | |

Table S5 The decay kinetics of PC[60]BM at different wavelength according to figure 9.

| PC[60]BM | | | | | | |
|---------------------------------|------------|------------|------------|------------|------------|-------------|
| λ(nm) | 452 | 498 | 617 | 725 | 880 | 1099 |
| A1 | 0.339 | 0.304 | 0.168 | 0.188 | 0.0774 | 0.0725 |
| τ1(ps) | 48.6 | 70.5 | 82.4 | 91.4 | 1.1 | 3.11 |
| A2 | 0.305 | 0.326 | 0.16 | 0.143 | 0.253 | 0.281 |
| τ2(ps) | 680 | 1060 | 1340 | 1010 | 40.9 | 58.8 |
| A3 | 0.355 | 0.37 | 0.672 | 0.669 | 0.552 | 0.507 |
| τ3(ps) | inf | inf | inf | inf | 1190 | 1160 |

Table S6 The decay kinetics of PC[70]BM at different wavelength according to figure 10.

| PC[70]BM | | | | |
|---------------------------------|------------|------------|------------|-------------|
| λ(nm) | 530 | 719 | 873 | 1092 |
| A1 | 0.4228 | 0.4255 | 0.3449 | 0.4723 |
| τ1(ps) | 104 | 136 | 31.7 | 22.8 |
| A2 | 0.221 | 0.199 | 0.4 | 0.25 |
| τ2(ps) | 646 | 972 | 495 | 1430 |
| A3 | 0.265 | 0.198 | 0.295 | 0.491 |
| τ3(ps) | inf | inf | inf | inf |