Analytic model for organic bulk heterojunction solar cells

based on Saha equation for exciton dissociation

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Electronic Supplementary Material (ESI)

I. Analytic solutions for drift-diffusion equations

In following paragraphs, we analytically solve current continuity equations in Eq. (2) for electrons and holes. Since we adopt the FD statistics, the boundary conditions for the carrier densities are as following forms

$$n(0) = \int_{-\infty}^{\infty} \frac{D_n(E)dE}{1 + exp[(E_g - W_{an} + E)/kT]} \qquad (S1a)$$

$$n(L) = \int_{-\infty}^{\infty} \frac{D_n(E)dE}{1 + exp[(W_{cat} + E)/kT]} \qquad (S1b)$$

$$p(0) = \int_{-\infty}^{\infty} \frac{D_p(E)dE}{1 + exp[(W_{an} - E)/kT]} \qquad (S2a)$$

$$p(L) = \int_{-\infty}^{\infty} \frac{D_p(E)dE}{1 + exp[(E_g - W_{cat} - E)/kT]} \qquad (S2b)$$

$D(E)$ is the Gaussian DOS with two parameters N_0 and σ. For an asymmetric device, N_0 and σ should take different values, N_{0n} and σ_n, N_{0p} and σ_p.

$$D(E) = (N_0/\sigma\sqrt{2\pi})exp(-E^2/2\sigma^2) \qquad (S3)$$

Three auxiliary densities n_1, p_1 and n_i needed in the SRH recombination rate Eq. (11) can be expressed as follows

$$n_1 = [n(0)n(L)]^{1/2}, \quad p_1 = [p(0)p(L)]^{1/2}, \quad n_i = (n_1 p_1)^{1/2} \qquad (S4)$$

The degenerate coefficients ζ_n and ζ_p can be solved by using following method. Under the quasi-equilibrium condition, the densities of electrons and holes can be expressed as

$$n = \int_{-\infty}^{\infty} \frac{D_n(E)dE}{1 + exp[(E - E_{Fn})/kT]} \qquad (S5a)$$

$$p = \int_{-\infty}^{\infty} \frac{D_p(E)dE}{1 + exp\left[(E_{Fp} - E)/kT\right]} \qquad (S5b)$$

Introducing alternative variables y_n and y_p

$$y_n = exp(E_{Fn}/kT), \quad y_p = exp(-E_{Fp}/kT) \qquad (S6)$$

Eq. ($S5$) can be changed to following algebraic equations about y_n and y_p

$$y_n = n \Big/ \int_{-\infty}^{\infty} \frac{D_n(E)dE}{y_n + exp(E/kT)} \qquad (S7a)$$

$$y_p = p \Big/ \int_{-\infty}^{\infty} \frac{D_p(E)dE}{y_p + exp(-E/kT)} \qquad (S7a)$$

The degenerate coefficients ζ_n and ζ_p can be expressed as

$$\zeta_n = \left(\frac{n}{kT}\right)\left(\frac{dn}{dE_{Fn}}\right)^{-1} = \frac{\displaystyle\int_{-\infty}^{\infty} \frac{D_n(E)dE}{y_n + exp(E/kT)}}{\displaystyle\int_{-\infty}^{\infty} \frac{exp(E/kT)D_n(E)dE}{[y_n + exp(E/kT)]^2}} \qquad (S8a)$$

$$\zeta_p = -\left(\frac{p}{kT}\right)\left(\frac{dp}{dE_{Fp}}\right)^{-1} = \frac{\displaystyle\int_{-\infty}^{\infty} \frac{D_p(E)dE}{y_p + exp(-E/kT)}}{\displaystyle\int_{-\infty}^{\infty} \frac{exp(E/kT)D_p(E)dE}{[y_p + exp(-E/kT)]^2}} \qquad (S8a)$$

The mobility function $\mu(F,p)$ used in this work is the improved expression of Sun et al.[45]

$$\mu(T,p,F) = \mu(T,p)f(T,F) \qquad (S9)$$

$$\mu(T,p) = \mu_0 c_1 exp\left(-c_2\hat{\sigma}^2\right)exp\left[\frac{1}{2}(\hat{\sigma}^2 - \hat{\sigma})\left(2p/N_0\right)^\delta\right] \qquad (S10)$$

$$c_1 = 1.8 \times 10^{-9}, \quad c_2 = 0.5268 - 0.384aN_0^{1/3} \qquad (S11)$$

$$\delta = 2\hat{\sigma}^{-2}\left[ln(\hat{\sigma}^2 - \hat{\sigma}) - ln(ln4)\right] \qquad (S12)$$

$$f(T,F) = exp\left\{0.44(\hat{\sigma}^{3/2} - 2.2)\left[\sqrt{1 + 80(eFa/\sigma)^2} - 1\right]\right\} \qquad (S13)$$

Substitution of Eqs. (7, 9, 12) into Eq (5) yields,

$$C_{n2}\frac{d^2n}{dx^2} + C_{n1}\frac{dn}{dx} - (1 - P)(k_n + g_n)n = -PG(x) - (1 - P)R_0 \qquad (S14a)$$

$$C_{p2}\frac{d^2p}{dx^2} - C_{p1}\frac{dp}{dx} - (1 - P)(k_p + g_p)p = -PG(x) - (1 - P)R_0 \qquad (S14b)$$

with $R_0 = R_{b0} + R_{t0}$. Eqs. ($S14$) are second order linear differential equations, and can be solved as follows

2

$$n(x) = A_{n1}e^{\delta_{n1}x} + A_{n2}e^{\delta_{n2}x} + f_n(x) \qquad (S15)$$

$$p(x) = A_{p1}e^{\delta_{p1}(L-x)} + A_{p2}e^{\delta_{p2}(L-x)} + f_p(x) \qquad (S16)$$

with following characteristic roots

$$\delta_n = (2C_{n2})^{-1}\left\{-C_{n1} \pm \left[C_{n1}^2 + 4(1-P)(k_n + g_n)C_{n2}\right]^{1/2}\right\} \qquad (S17a)$$

$$\delta_p = (2C_{p2})^{-1}\left\{C_{p1} \pm \left[C_{p1}^2 + 4(1-P)(k_p + g_p)C_{p2}\right]^{1/2}\right\} \qquad (S17a)$$

and special solutions of inhomogeneous equations

$$f_n(x) = R_0/(k_n + g_n) + \int_{\lambda_1}^{\lambda_2} \left[B_{n1}(\lambda)e^{-\eta(\lambda)x} + B_{n2}(\lambda)e^{-\eta(\lambda)(2L-x)}\right]I_0(\lambda)\eta(\lambda)d\lambda \quad (S18a)$$

$$f_p(x) = R_0/(k_p + g_p) + \int_{\lambda_1}^{\lambda_2} \left[B_{p1}(\lambda)e^{-\eta(\lambda)x} + B_{p2}(\lambda)e^{-\eta(\lambda)(2L-x)}\right]I_0(\lambda)\eta(\lambda)d\lambda \quad (S18b)$$

In calculations, we follows from Kim et al.[42] to take $\lambda_1 = 300$ nm, $\lambda_2 = 1100$ nm, and normalized the incident light intensity P_{in} as 850 W/m^2.

$$B_{n1} = -P\left[\eta^2(\lambda)C_{n2} - \eta(\lambda)C_{n1} - (1-P)(k_n + g_n)\right]^{-1} \qquad (S19a)$$

$$B_{n2} = -P\left[\eta^2(\lambda)C_{n2} + \eta(\lambda)C_{n1} - (1-P)(k_n + g_n)\right]^{-1} \qquad (S19b)$$

$$B_{p1} = -P\left[\eta^2(\lambda)C_{p2} + \eta(\lambda)C_{p1} - (1-P)(k_p + g_p)\right]^{-1} \qquad (S20a)$$

$$B_{p2} = -P\left[\eta^2(\lambda)C_{p2} - \eta(\lambda)C_{p1} - (1-P)(k_p + g_p)\right]^{-1} \qquad (S20b)$$

The coefficients A_{n1}, A_{n2}, A_{p1} and A_{p2} can be determined from the boundary conditions in Eqs. ($S1$, $S2$), the solved expressions are as follows

$$A_{n1} = \frac{[n(0) - f_n(0)]exp(\delta_{n2}L) - n(L) + f_n(L)}{exp(\delta_{n2}L) - exp(\delta_{n1}L)} \qquad (S21a)$$

$$A_{n2} = \frac{[n(0) - f_n(0)]exp(\delta_{n1}L) - n(L) + f_n(L)}{exp(\delta_{n1}L) - exp(\delta_{n2}L)} \qquad (S21b)$$

$$A_{p1} = \frac{[p(L) - f_p(L)]exp(\delta_{p2}L) - p(0) + f_p(0)}{exp(\delta_{p2}L) - exp(\delta_{p1}L)} \qquad (S22a)$$

$$A_{p2} = \frac{[p(L) - f_p(L)]exp(\delta_{p1}L) - p(0) + f_p(0)}{exp(\delta_{p1}L) - exp(\delta_{p2}L)} \qquad (S22b)$$
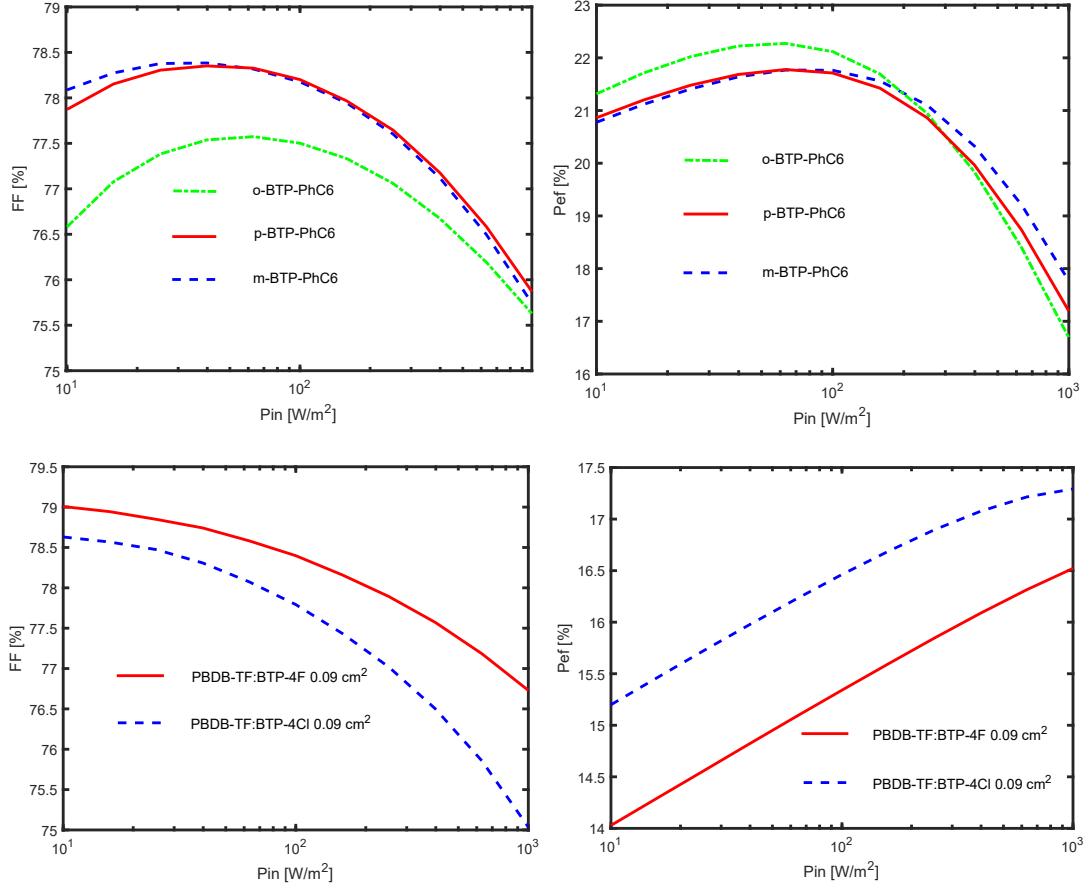
II. Additional figures

Fig. S1 Variations of *FF* and P_{ef} versus light intensity P_{in} for five OSCs with different materials, lines – theoretical curves with parameters in Table 1, symbols – experimental data: (a) and (b) *FF* - P_{in} and P_{ef} - P_{in} curves for m-BTP-PhC6, o-BTP-PhC6 and p-BTP-PhC6 materials, respectively[10]; (c) and (d) *FF* - P_{in} and P_{ef} - P_{in} curves for BTP-4Cl and BTP-4F materials, respectively[6].
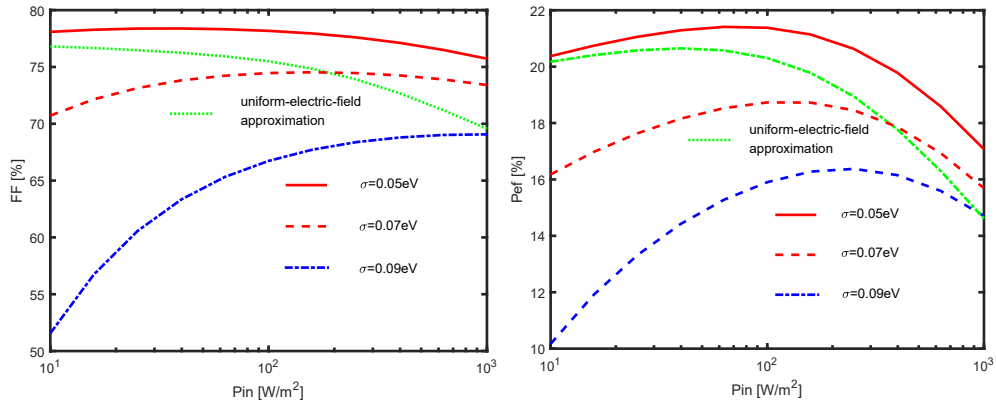

Fig. S2 Variations of *FF* and P_{ef} versus light intensity P_{in} for the OSC with m-BTP-PhC6 material, lines – theoretical curves with other parameters in Table 1 and σ = 0.05, 0.07, 0.09 eV, dot line - theoretical curve with σ = 0.05 eV and not considering SCLC effect (UEFA), respectively. (a) *FF* - P_{in} curves, (b) P_{ef} - P_{in} curves.
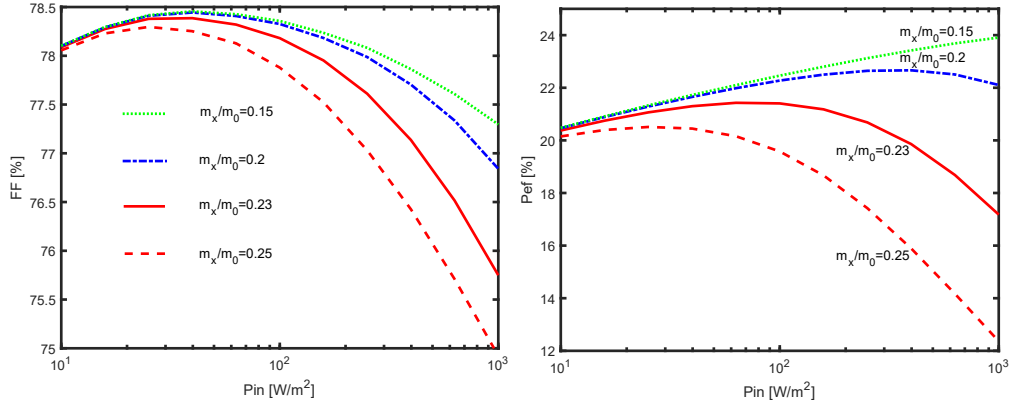
Fig. S3 Variations of *FF* and P_{ef} versus light intensity P_{in} for the OSC with m-BTP-PhC6 material, lines – theoretical curves with other parameters in Table 1 and $m_x / m_0 = 0.15, 0.2, 0.23, 0.25$, respectively. (a) *FF* - P_{in} curves, (b) P_{ef} - P_{in} curves.
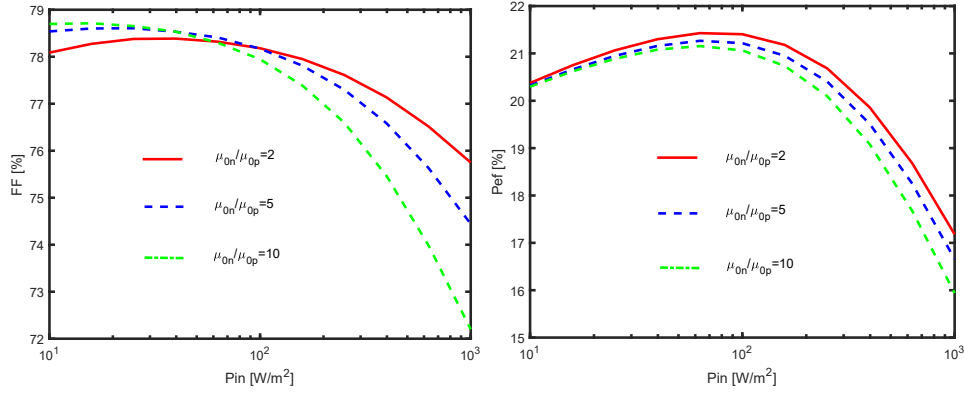

Fig. S4 Variations of *FF* and P_{ef} versus light intensity P_{in} for the OSC with m-BTP-PhC6 material, lines – theoretical curves with other parameters in Table 1 and with fixed ($\mu_{0n}+\mu_{0p}$) and ratio μ_{0n}/μ_{0p} = 2, 5, 10, respectively. (a) *FF* - P_{in} curves, (b) P_{ef} - P_{in} curves.
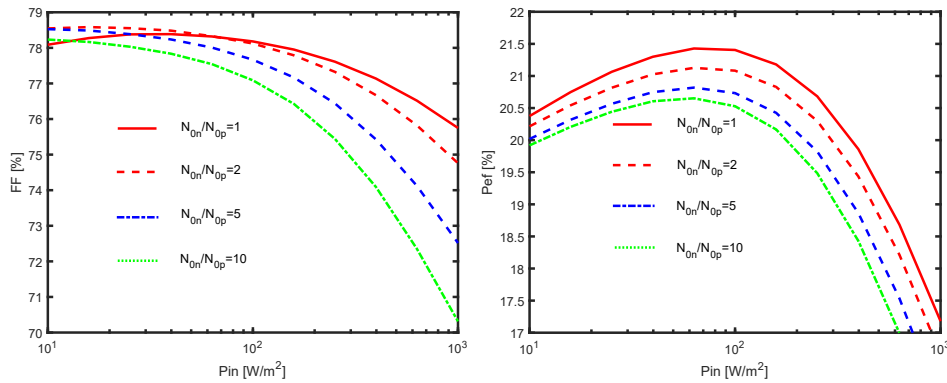

Fig. S5 Variations of *FF* and P_{ef} versus light intensity P_{in} for the OSC with m-BTP-PhC6 material, lines – theoretical curves with other parameters in Table 1 and with fixed ($N_{0n}+N_{0p}$) and ratio N_{0n}/N_{0p} = 1, 2, 5, 10, respectively. (a) *FF* - P_{in} curves, (b) P_{ef} - P_{in} curves.

Fig. S6 Variations of *FF* and P_{ef} versus light intensity P_{in} for the OSC with m-BTP-PhC6 material, lines – theoretical curves with other parameters in Table 1 and with fixed ($W_{an}+W_{cat}$) and ratio W_{an}/W_{cat} = 0.5, 0.157/0.15, 2, 3, respectively. (a) *FF* - P_{in} curves, (b) P_{ef} - P_{in} curves.
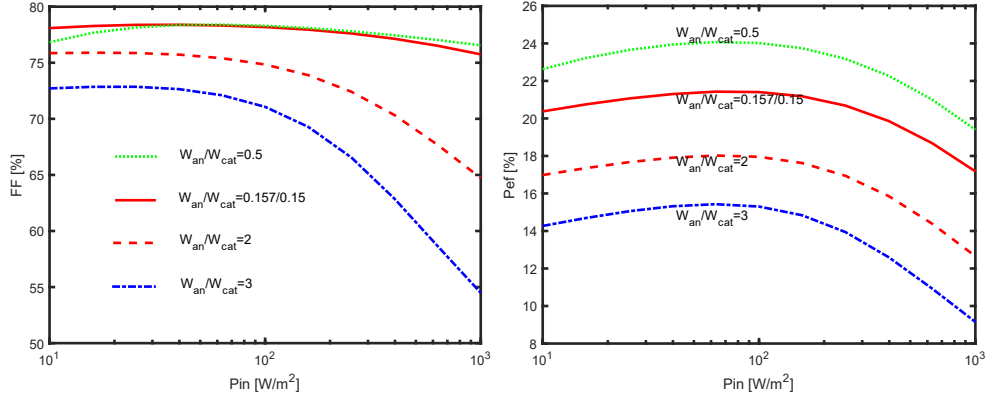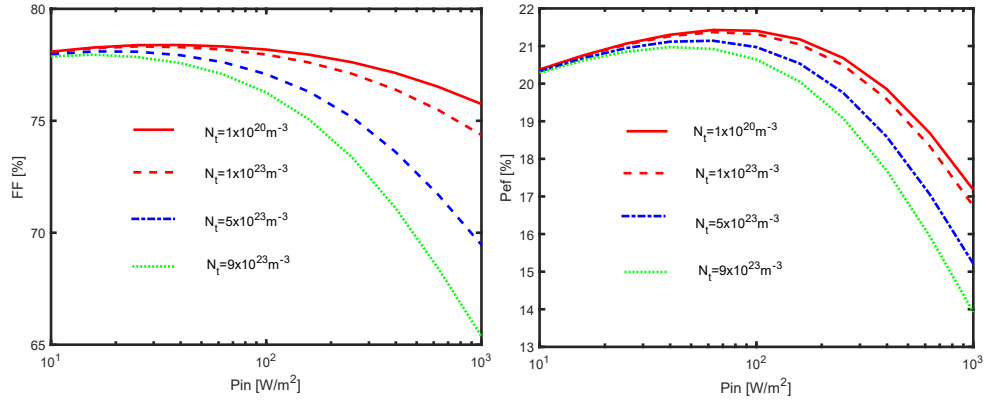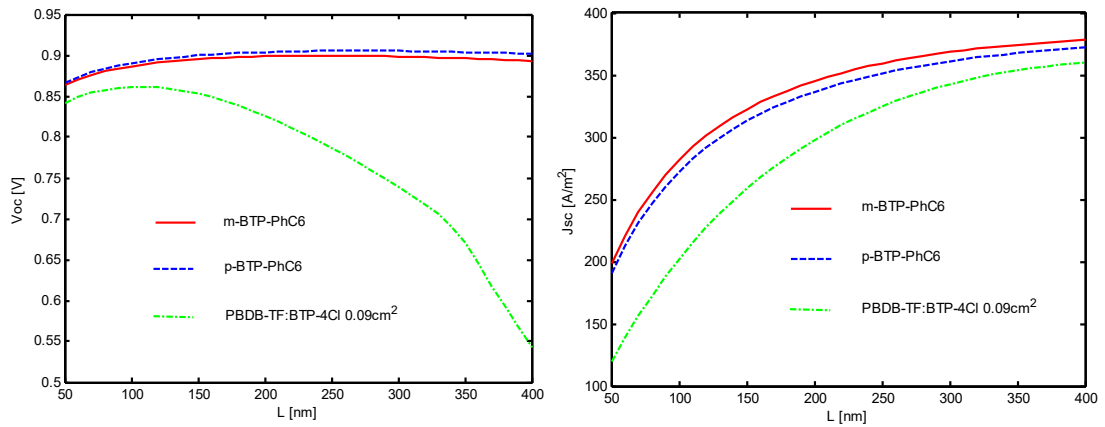

Fig. S7 Variations of *FF* and P_{ef} versus light intensity P_{in} for the OSC with m-BTP-PhC6 material, lines – theoretical curves with other parameters in Table 1 and with N_t = 1×10^{20} , 1×10^{23}, 5×10^{23}, 9×10^{23} m^{-3}, respectively. (a) *FF* - P_{in} curves, (b) P_{ef} - P_{in} curves.
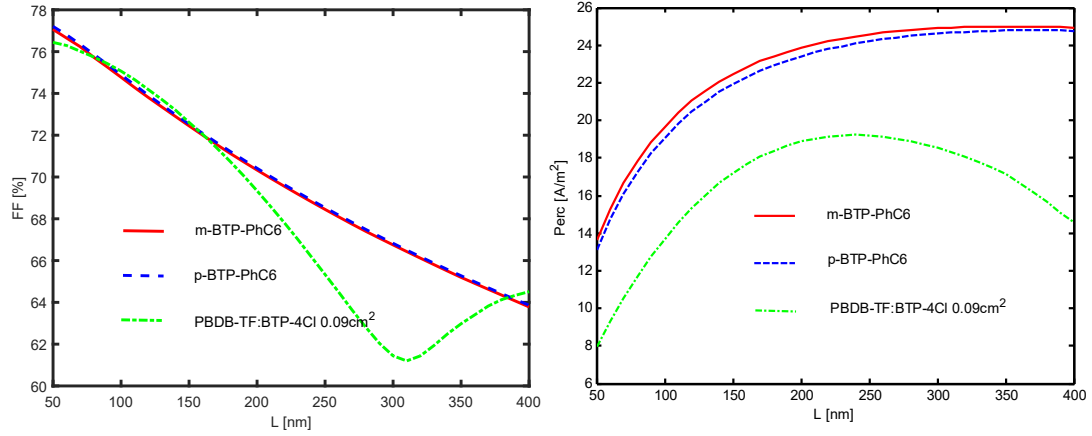
Fig. S8 Variations of performance parameters versus thickness *L* of active layer for three OSCs with m-BTP-PhC6, p-BTP-PhC6, and PBDB-TF: BTP-4Cl materials, lines – theoretical curves with parameters in Table 1, respectively. (a) V_{oc} - *L* curves, (b) J_{sc} - *L* curves, (c) *FF* - *L* curves, (d) P_{ef} - *L* curves.

III. Predicted J-V curves for 15 compounds listed in Table 2
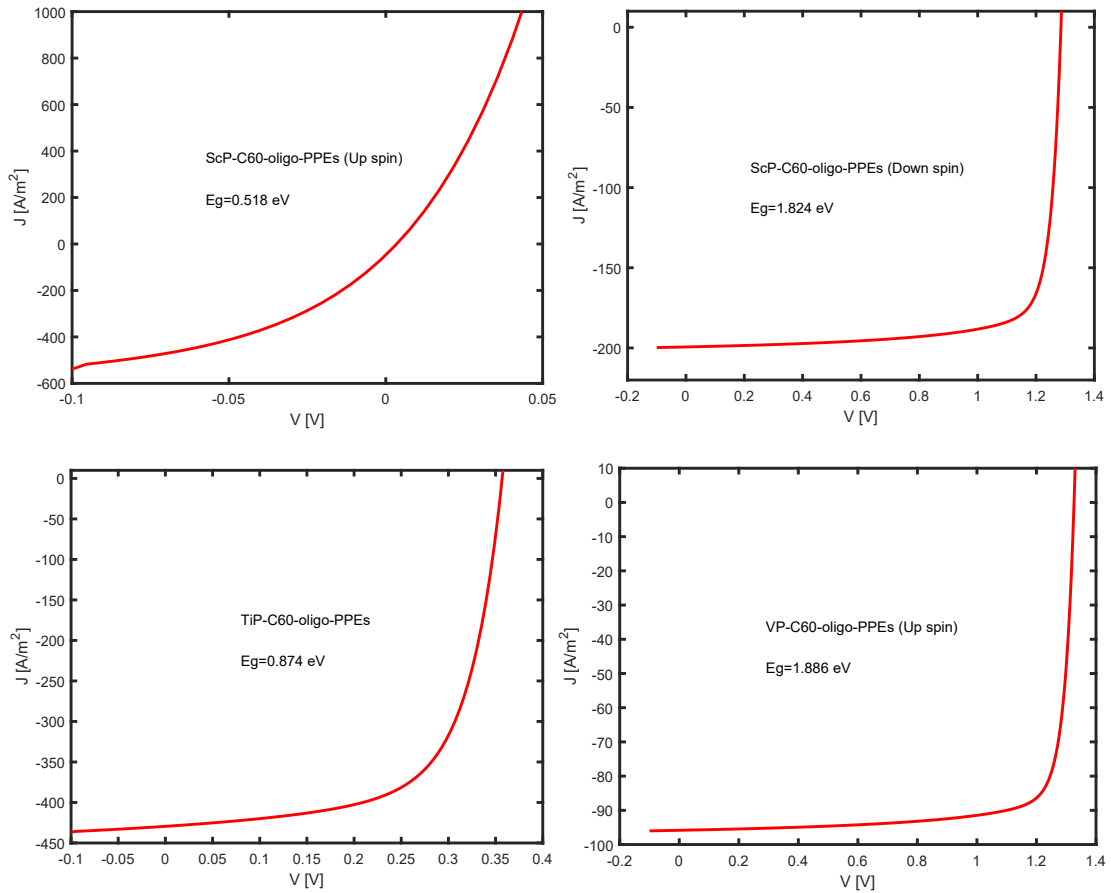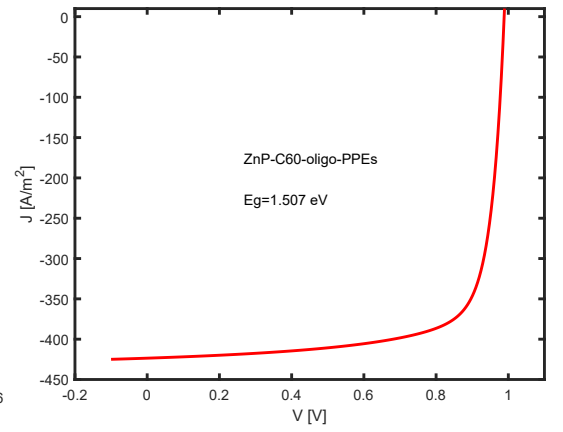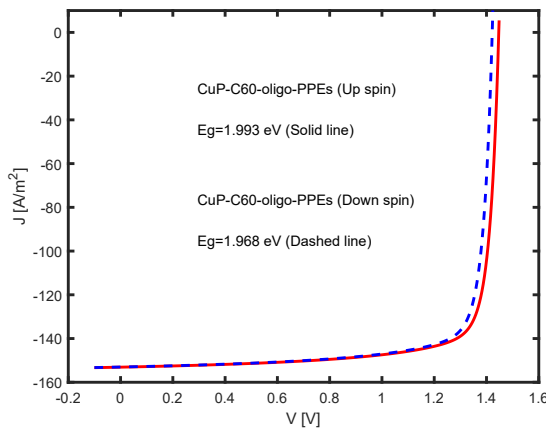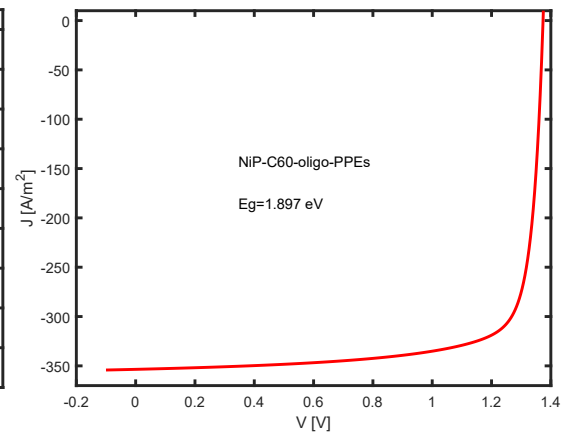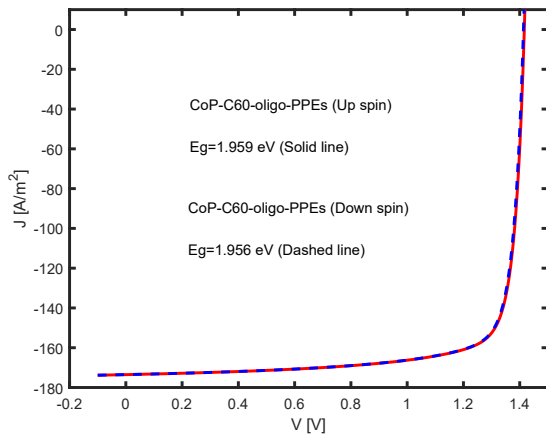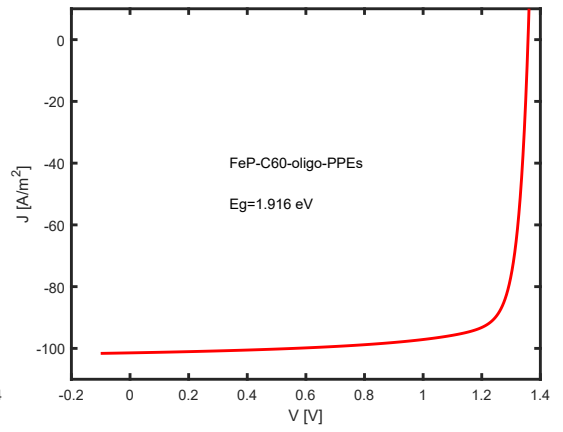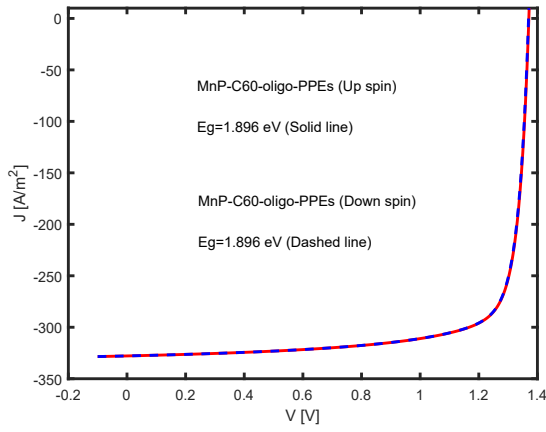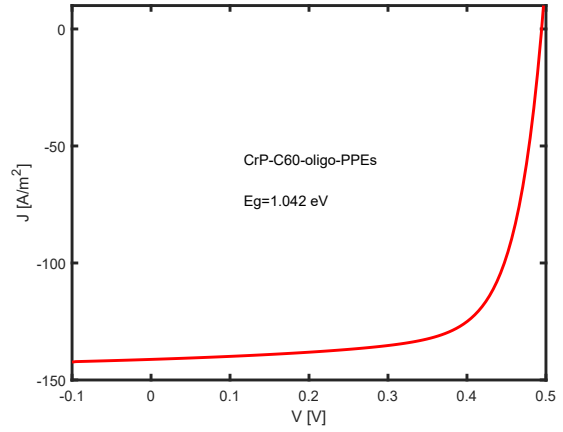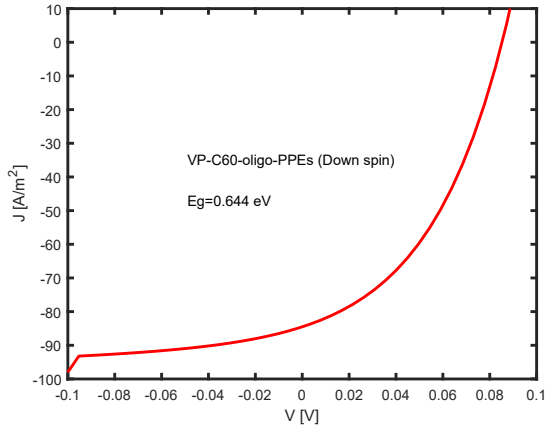
IV. MATLAB codes for calculations of J-V curves

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%
        %%                                              %%
        %%    MATLAB codes of DDM model for J-V curve of OSCs    %%
        %%               Main Program                   %%
        %%                                              %%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%

    clear all;
%     close all;

% Defining the Fundamental Constants %
    q        = 1.6021892E-19;              % C or [J/eV]
    kb       = 1.380662E-23;               % [J/K]
    m0       = 9.10938188E-31;             % [kg] Mass of electron
    me       = 0.198*m0;                   % [kg] Efective mass of electron
    epsr     = 3.0;                        % Relative permittivity at T
    eps      = epsr*8.854187817E-12;       % [F/m] This includes the epsr = 3
    T        = 300;                        % [K]
    Vt       = kb*T/q;                     % [eV]
    h        = 6.626068E-34;               % [J*s] Plank constant
    cc       = 2.99792458E8;               % [m/s] Velocity of light
```

% Data for Optical Absorption in OSC read from PTQ10:m-BTP-PhC6 of Fig.S2 [Gaoda Chai et al. Energy Environ. Sci., 2021, 14, 3469-3479];

```
    xpic=[194 211 230 234 250 267 283 298 308 314 319 323 330 336 343 349 362 381 400 419
433 448 461 474 486 497 508 518 530 538 547 555 566 576 588 601 610 623 636 653 ...
        664 676 692 699 708 715 727 738 743 747 750 753 758 762 768 773 780 791 815 845
866 885 906 928 950 974 995 1020 1045 1068 1089 1099 1110 ...
        1117 1125 1133 1138 1143 1149 1157 1164 1173 1181 1190 1197 1209 1222 1237
1255 1274 1298 1327 1354 1388 1419 1443 1472 1508 1523 1548 1576 1600]; % Data points
from REF
    ypic=[973 852 738 573 540 520 562 548 573 598 625 650 686 711 743 771 803 823 838 834
825 806 783 757 727 698 668 641 611 583 555 528 505 477 450 419 393 363 341 336 ...
```

351 364 348 323 295 269 250 270 298 322 350 376 408 435 465 498 529 554 562 551
527 506 479 456 436 417 400 373 343 326 335 355 376 403 ...
          430 465 494 518 547 580 614 649 678 704 740 766 799 827 858 882 901 915 923 933
939 944 947 959 963 967 970 973]; % Data points from REF
     xs=350+(1050-350)*(xpic-283)/(1510-283);   % [nm]
     yr=0+(1-0)*(ypic-973)/(250-973);   % Normalized absorption (%) for 350-
1050 nm
     ys=2.0E7*yr;   % [to 1/m]
% Data for absorption spectrum end

     AM1dot5   = xlsread('AM0AM1_5.xls');   % read data of solar spectrum
     wl   = (AM1dot5(43:941,1))';   % [nm]
     cas   = interp1(xs,ys,wl,'linear');   % [1/m] Absorption spectrum
     Ipa   = (AM1dot5(43:243,3))';   % [W/m^2/nm] Incident-light power
density
     Ipb   = (AM1dot5(244:941,3))';   % [W/m^2/nm] Incident-light power
density
     Ipd   = [0.5*Ipa Ipb];
     Ipf   = Ipd.*(wl*1.0E-9/h/cc);   % [1/m^2/s] Incident photon flux, Step
of wave-length is 0.5 nm
     Ipt0   = sum(Ipd)   % [W/m^2] Total Incident-light
power density

% Defining the Material Constants %
     CN   = sqrt(2*pi);   % normalizing coefficient for Gauss
DOS
     N0n   = 1.0E26;   % [1/m^3] Prefactor in Gauss DOS
     N0p   = 1.0E26;   % [1/m^3] Prefactor in Gauss DOS
     Nt   = 1.0E20;
     sgm   = 0.05;   % [eV] Width of Gauss DOS for
carriers
     Em   = 10*sgm;
     dE   = sgm/10;
     Ed   = -Em:dE:Em;   % [eV] (E-Ev), Energy variable in
Gauss DOS
     GSn   = N0n/CN/sgm*exp(-0.5*(Ed/sgm).^2); % Gauss DOS
     GSp   = N0p/CN/sgm*exp(-0.5*(Ed/sgm).^2); % Gauss DOS

     al   = 3.0E-10;   % [m] Latice constant
     af   = 1/al;
     mu0   = 1.0E3;

%   Defining Effective Density of States %
     Eg   = 1.43;   % [eV] Band gap

```
Wan          = 0.157;                                    % [eV]
Wcat         = 0.15;                                     % [eV]
Vbi          = Eg-Wan-Wcat;


nan          = dE*sum(GSn./(1+exp((Ed+Eg-Wan)/Vt)));
ncat         = dE*sum(GSn./(1+exp((Ed+Wcat)/Vt)));
pan          = dE*sum(GSp./(1+exp((Wan-Ed)/Vt)));
pcat         = dE*sum(GSp./(1+exp((Eg-Wcat-Ed)/Vt)));


n1           = sqrt(nan*ncat);
p1           = sqrt(pan*pcat);
ni           = sqrt(n1*p1);
Nc           = sqrt(N0n*N0p)*exp(0.5*(sgm/Vt)^2)


gm           = 1.0;                       % Coefficient for generation rate
Pin          = 1000;                      % [W/m^2] Incident-light power
density
%      Pin        = Pind(ipin);            % [W/m^2] Incident-light power
density
kin          = Pin/Ipt0;
Ipd          = kin*[0.5*Ipa Ipb];
Ipf          = Ipd.*(wl*1.0E-9/h/cc);      % [1/m^2/s] Incident photon flux, Step
of wave-length is 0.5 nm


tn           = 1.0E-5;                     % SRH life time of electron
tp           = 1.0E-5;                     % SRH life time of hole
mun0         = 1.0E3;                      % [m2/V-s] Electron Mobility
mup0         = 5.0E2;                      % [m2/V-s] Hole Mobility
np0          = 1.0E50;                     % Parameter in Mobility
tx           = 2.0E-9;                     % Lifetime of exiton


% End of Definition of Material_Constants and some material constants

% Setting the size of the simulation %

xmx          = 80.0E-9;                    % [m]
nmx          = 80;
dx           = xmx/(nmx-1);
xd           = 0:dx:xmx;                   % Coordinate points


nd(1)        = nan;
nd(nmx)      = ncat;
pd(1)        = pan;
pd(nmx)      = pcat;
```

```
    for i=1:nmx
    Gx(i)        = sum((exp(-cas*xd(i))+exp(-cas*(2*xmx-xd(i)))).*Ipf.*cas);
    end
    G0           = mean(Gx);


    lmD          = sqrt(eps*Vt/q/G0/tx);
    Ex           = 13.6*me/m0/epsr^2
    AT           = (2*pi*m0*kb*T/h/h)^1.5*exp(-Ex/Vt);
    PX           = AT/2/G0/tx*(-1+sqrt(1+4*G0*tx/AT));
```

%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%   %%
%%   NON-EQUILIBRIUM   SOLUTION PART BEGINS   %%
%%   %%
%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

```
    Vmn          = -0.1;                         % [V]
    Vmx          = 1.1;                          % [V]
    nmxv         = 220;
    dV           = Vmx/nmxv;


    Ef           = (Vmn - Vbi)/xmx;                % [V/m] Strength of electric field
    An1          = nd(1)/(1-exp(Ef*xmx/Vt));
    An2          = nd(nmx)/(1-exp(Ef/Vt*xmx));
    Ap1          = pd(nmx)/(1-exp(Ef*xmx/Vt));
    Ap2          = pd(1)/(1-exp(Ef*xmx/Vt));

%    Initialize nd and pd
    nd           = An1*(1-exp(Ef*(xmx-xd)/Vt))-An2*(exp(Ef*xmx/Vt)-exp(Ef/Vt*(xmx-xd)));
    pd           = Ap1*(1-exp(Ef*xd/Vt))-Ap2*(exp(Ef*xmx/Vt)-exp(Ef/Vt*xd));
    nv           = mean(nd);                      % Estimate nv
    pv           = mean(pd);                      % Estimate pv

%    Calculate the Mobility at each Node
    for i=1:nmx
    mun(i)       = MoPSV(N0n,sgm,mun0,al,T,Ef,nd(i));
    mup(i)       = MoPSV(N0p,sgm,mup0,al,T,Ef,pd(i));
    end

    yn           = 1+0*xd;
    yp           = 1+0*xd;
```

```matlab
stn         = 1+0*xd;
stp         = 1+0*xd;
Cn1         = mean(mun*Ef);
Cn2         = Vt*mean(stn.*mun);
Cp1         = mean(mup*Ef);
Cp2         = Vt*mean(stp.*mup);

Vplot       = [];
Jplot       = [];
for Va = Vmn:dV:Vmx;                          % [V] Start Va increment for loop
Va
Ef          = (Va-Vbi)/xmx;                   % [V/m] Strength of electric field
Efx         = Ef+0*xd;

for js=1:10                                    % Start loop for self-consistency
tn          = eps/q/Nt./mun;
tp          = eps/q/Nt./mup;
nv          = mean(nd);
pv          = mean(pd);
mdv         = mean(nd.*pd.*(mun+mup));
kn          = q/eps*mdv/nv;
kp          = q/eps*mdv/pv;

gv          = mean(ni^2./(tp.*(nd+n1)+tn.*(pd+p1)));
npv         = mean(nd.*pd./(tp.*(nd+n1)+tn.*(pd+p1)));
gn          = npv/nv;
gp          = npv/pv;

gnv         = (1-PX)*(kn+gn);
gpv         = (1-PX)*(kp+gp);
wnt         = sqrt(Cn1^2+4*gnv*Cn2);
wpt         = sqrt(Cp1^2+4*gpv*Cp2);

dtn1        = (-Cn1-wnt)/2/Cn2;
dtn2        = (-Cn1+wnt)/2/Cn2;
dtp1        = (-Cp1-wpt)/2/Cp2;
dtp2        = (-Cp1+wpt)/2/Cp2;

Bn1         = -gm./(Cn2*cas.^2-Cn1*cas-gnv);
Bn2         = -gm./(Cn2*cas.^2+Cn1*cas-gnv);
Bp1         = -gm./(Cp2*cas.^2+Cp1*cas-gpv);
Bp2         = -gm./(Cp2*cas.^2-Cp1*cas-gpv);

%    Calculate gn, gn1, gp, gp1
```

```matlab
    for i=1:nmx
        gn(i)    = gv/gnv+PX*sum((Bn1.*exp(-cas*xd(i))+Bn2.*exp(-cas*(2*xmx-xd(i)))).*Ipf.*cas);
        gn1(i)   = PX*sum((-Bn1.*exp(-cas*xd(i))+Bn2.*exp(-cas*(2*xmx-xd(i)))).*Ipf.*cas.^2);
        gp(i)    = gv/gpv+PX*sum((Bp1.*exp(-cas*xd(i))+Bp2.*exp(-cas*(2*xmx-xd(i)))).*Ipf.*cas);
        gp1(i)   = PX*sum((-Bp1.*exp(-cas*xd(i))+Bp2.*exp(-cas*(2*xmx-xd(i)))).*Ipf.*cas.^2);
    end


    An1        = ((nd(1)-gn(1))*exp(dtn2*xmx)-nd(nmx)+gn(nmx))/(exp(dtn2*xmx)-exp(dtn1*xmx));
    An2        = ((nd(1)-gn(1))*exp(dtn1*xmx)-nd(nmx)+gn(nmx))/(exp(dtn1*xmx)-exp(dtn2*xmx));
    Ap1        = ((pd(nmx)-gp(nmx))*exp(dtp2*xmx)-pd(1)+gp(1))/(exp(dtp2*xmx)-exp(dtp1*xmx));
    Ap2        = ((pd(nmx)-gp(nmx))*exp(dtp1*xmx)-pd(1)+gp(1))/(exp(dtp1*xmx)-exp(dtp2*xmx));

%    Calculate nd, nd1, pd, pd1
    nd         = An1*exp(dtn1*xd)+An2*exp(dtn2*xd)+gn;
    nd1        = An1*dtn1*exp(dtn1*xd)+An2*dtn2*exp(dtn2*xd)+gn1;           %
derivative of nd to x
    pd         = Ap1*exp(dtp1*(xmx-xd))+Ap2*exp(dtp2*(xmx-xd))+gp;
    pd1        = -Ap1*dtp1*exp(dtp1*(xmx-xd))-Ap2*dtp2*exp(dtp2*(xmx-xd))+gp1;   %
derivative of pd to x

%    Calculate Jn, Jnv, Jp, Jpv
    Jnv        = q*nd*Cn1+q*Cn2*nd1;
    Jpv        = q*pd*Cp1-q*Cp2*pd1;
    Jtv        = mean(Jnv+Jpv);

%        yn         = 0*xd;
%        yp         = 0*xd;
    for j=1:5
        for i=1:nmx
            yn(i)    = nd(i)/(dE*sum(GSn./(yn(i)+exp(Ed/Vt))));
            yp(i)    = pd(i)/(dE*sum(GSp./(yp(i)+exp(-Ed/Vt))));
        end
    end
    for i=1:nmx
        stn(i)    = sum(GSn./(yn(i)+exp(Ed/Vt)))/sum(GSn.*exp(Ed/Vt)./(yn(i)+exp(Ed/Vt)).^2);
```

```matlab
        stp(i)      = sum(GSp./(yp(i)+exp(-Ed/Vt)))/sum(GSp.*exp(-Ed/Vt)./(yp(i)+exp(-Ed/Vt))).^2);
    end

    for i=1:nmx
    mun(i)      = MoPSV(N0n,sgm,mun0,al,T,Efx(i),nd(i));
    mup(i)      = MoPSV(N0p,sgm,mup0,al,T,Efx(i),pd(i));
    end

    Jn          = q*Efx.*nd.*mun+kb*T*stn.*mun.*nd1;
    Jp          = q*Efx.*pd.*mup-kb*T*stp.*mup.*pd1;
    Jt          = mean(Jn+Jp);                                      % total
photocurrent

    Edx         = 0*xd;
    for i=2:nmx
        Edx(i)      = Edx(i-1)+q/eps*dx*pd(i-1);
    end
    Ef1         = (Va-Vbi)/xmx-dx/xmx*sum(Edx);
    Efx         = Ef1+Edx;

    Cn1         = mean(mun.*Efx.*nd)/mean(nd);
    Cn2         = Vt*mean(stn.*mun.*nd1)/mean(nd1);
    Cp1         = mean(mup.*Efx.*pd)/mean(pd);
    Cp2         = Vt*mean(stp.*mup.*pd1)/mean(pd1);

%      erj          = 100*abs(Jt./Jtv-1)
    end                              % end of loop for js in line 158

    erj         = 100*abs(Jt./Jtv-1)
    Vplot       = [Vplot,Va];
    Jplot       = [Jplot,Jt];

%      figure(3)
%      plot(xd, mun,'--b',xd,mup,'--b','LineWidth',2); hold on;
%      figure(4)
%      plot(xd, stn,'--b',xd,stp,'--b','LineWidth',2); hold on;
%      figure(5)
%      plot(xd, Jtv,'or',xd,Jt,'+b','LineWidth',2); hold on;
%      figure(6)
%      plot(xd, nd,'-r',xd,pd,'--b','LineWidth',2); hold on;
%      figure(6)
%      plot(xd, Efx,'-r','LineWidth',2); hold on;
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%              END OF NON-EQUILIBRIUM    SOLUTION PART
%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

end                    % Loop for Va

   figure(9)
   plot(Vplot, Jplot,'-r','LineWidth',2); hold on;
   axis([0 1.2 -300 10]);
   xlabel('V [V]');
   ylabel('J [A/m^2]');
   title('J vs V');


%    Following data read from [Fine-tuning of side-chain orientations on nonfullerene acceptors enables
%    organic solar cells with 17.7% efficiency, Gaoda Chai et al. Energy Environ. Sci. 14, 3469 (2021)]
%      Vfig=[431 493 557 621 685 748 811 875 940 1004 1067 1131 1195 1258 1322 1386 1450 1515 1554 1578 1608];          % PTQ10:o-BTP-PhC6
%      Jfig=[987 985 985 985 982 980 980 978 975 972 969 964 962 954 944 923 879 754 580 414 131];                      % PTQ10:o-BTP-PhC6
%
     Vfig=[431 493 557 621 685 748 811 875 940 1004 1067 1131 1195 1258 1322 1386 1450 1491 1515 1538 1554];          % PTQ10:m-BTP-PhC6
     Jfig=[1082 1082 1080 1079 1078 1077 1076 1074 1070 1068 1066 1061 1060 1050 1038 1007 915 756 598 339 131];     % PTQ10:m-BTP-PhC6
%
%      Vfig=[431 493 557 621 685 748 811 875 940 1004 1067 1131 1195 1258 1322 1386 1450 1492 1515 1544 1561];          % PTQ10:p-BTP-PhC6
%      Jfig=[1057 1056 1055 1055 1053 1052 1049 1047 1045 1043 1038 1037 1030 1023 1011 984 904 768 636 351 131];      % PTQ10:p-BTP-PhC6

     Vexp=0+0.8*(Vfig-431)/(1450-431);                          %  Unit [V]
     Jexp=10*(-25+25*(Jfig-1070)/(132-1070));                   % Unit from [mA/cm^2] to [A/m^2]
%    Above data read from [Fine-tuning of side-chain orientations on nonfullerene acceptors enables
%    organic solar cells with 17.7% efficiency, Gaoda Chai et al. Energy Environ. Sci. 14, 3469 (2021)]
```

```
    figure(9)
    plot(Vexp, Jexp,'or','LineWidth',2); hold on;

    Ipt          = sum(Ipd)                                        %
[W/m^2] Total Incident-light power density
```

```
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%
        %%                                              %%
        %%        Subprogram for Improved Pasveer Mobility Model    %%
        %%        Dependent to temperature, density and electric field    %%
        %%                                              %%

%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%%%%%%%%%%%%%%%%%%%%%%%%

    function MoPSV=MoPSV(N0,sgm,mu0,al,T,E,P)
    C0    = 0.5+0.5*sqrt(1+4*log(4));

    SG    = sgm;      M0 = mu0;      A = 10*al;
    C1    = 1.8E-9;
%       C2    = 0.42;
    C2    = 0.5268-0.384*al*N0.^(1/3);

    SM    = 1.60217653/1.3806505*10000*SG/T;
    SM2 = SM*SM;
    MT0 = M0*C1*exp(-C2*SM2);
    if (SM<C0)
    DL    = 0;
    else
    DL    = 2/SM2*(log((SM2-SM)/log(4)));
    end
%       PAD = exp(DL*log(2*P/N0));
    PAD = real((2*P/N0)^DL);
    MTP = MT0*exp(0.5*(SM2-SM)*PAD);

    EAS = sqrt(1+0.8*(E*A/SG)^2)-1;
    FTE = exp(0.44*(SM*sqrt(SM)-2.2)*EAS);
    MoPSV = MTP*FTE;
end
```