Electronic Supporting Information

Enhanced Performance in Low Band Gap Polymer Solar Cells via Lattice Surface Resonance of Non-Noble Metals

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S1 Simulation materials

In order to model the simulation materials, the optical constants of ITO, TiO_2, PTB7:$PC_{71}BM$,MoO_3, and metal electrode (Ag) were implemented in FDTD using the multi-coefficient model (MCM), which is a generalized dispersive material model. This model provides much better fits to experimental data than conventional models like Drude and/or Lorentz. The MCM employs a rational function with multiple optimized poles, enabling extremely accurate broadband fitting of experimental n and k data while maintaining causality and numerical stability. This approach is particularly suitable for organic semiconductors and metal oxides with complex dispersion, ensuring reliable optical simulations across the entire solar spectrum.

S2 Power conversion Efficiency Calculation

The PCE of the devices was calculated as follows. The open circuit (V_{oc}) was calculated using Equation1.

$$V_{\mathrm{oc}} = \frac{1}{q}\left|E_{\mathrm{HOMO}}^{\mathrm{Donor}} - E_{\mathrm{LUMO}}^{\mathrm{Acceptor}}\right| - 0.3\,\mathrm{V} \tag{1}$$

Here, the HOMO of PTB7 and LUMO of $PC_{71}BM$ energy levels are -5.15 eV and -3.9 eV to 4.0 eV, the potential energy difference at the donor/acceptor interface is 0.85 V.

The fill factor (FF) of the simulated devices is calculated using Equation 2, and the calculated to be 0.70%.

$$\mathrm{FF} = \frac{(V_{oc} - \ln(V_{oc} + 0.72))}{(V_{oc} + 1)} \tag{2}$$

The short-circuit current density (J_{sc}) is calculated using Equation3.

$$J_{\mathrm{sc}} = q \int_{300\,\mathrm{nm}}^{1000\,\mathrm{nm}} \mathrm{A}(\lambda)\, \frac{\lambda}{hc}\, \mathrm{AM1.5G}(\lambda)\, d\lambda \tag{3}$$

Where AM1.5G is the solar irradiance spectrum, $\mathrm{A}(\lambda)$ is optical absorption in the AL of the devices and determined from the time-averaged optical absorption power in the absorber layer as estimated in Equation **??** using FDTD simulation.

$$P_{\mathrm{abs}} = \frac{1}{2}\, \varepsilon_0\, \omega \int \mathrm{Im}(\varepsilon)\, |\mathbf{E}|^2\, dV \tag{4}$$

Where ε'' is the imaginary part of permittivity for the absorber layer electric field amplitude E is the electric field in the AL,ω is the angular frequency of the incident light, and V is the volume of the AL materials.

Finally, the PCE was calculated using Equation 5

$$\mathrm{PCE} = \frac{J_{\mathrm{sc}}\, V_{\mathrm{oc}}\, \mathrm{FF}}{P_{\mathrm{in}}}, \tag{5}$$

S3 Supplementary Figures and Tables

Put all table belwo

S4 References

References

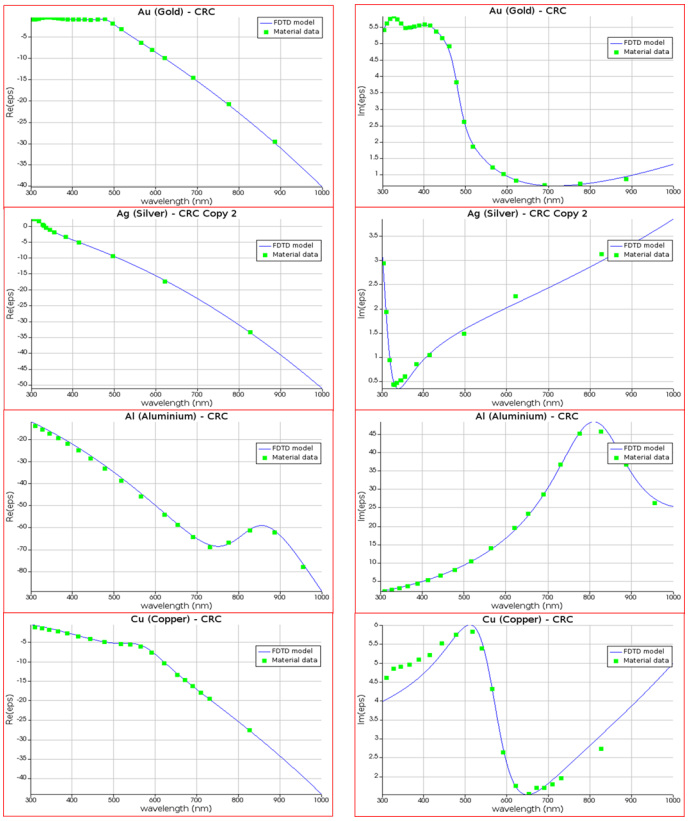

Figure S1: Material dispersion of plasmonic particles (Ag, Al, Au and Cu) fitted using the multi-coefficient model (MCM) in FDTD. The MCM provides accurate broadband reproduction of the experimental refractive index (n) and extinction coefficient (k) data.

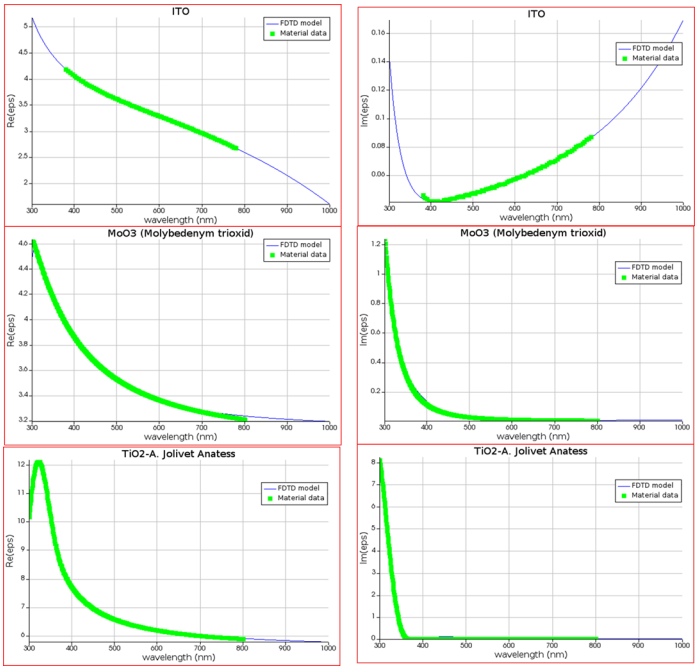

Figure S2: The fitted curves are given by the multi-coefficient model (MCM) in FDTD of ITO, MoO_3, TiO_2 over the solar spectrum range from 300 nm to 1000 nm.

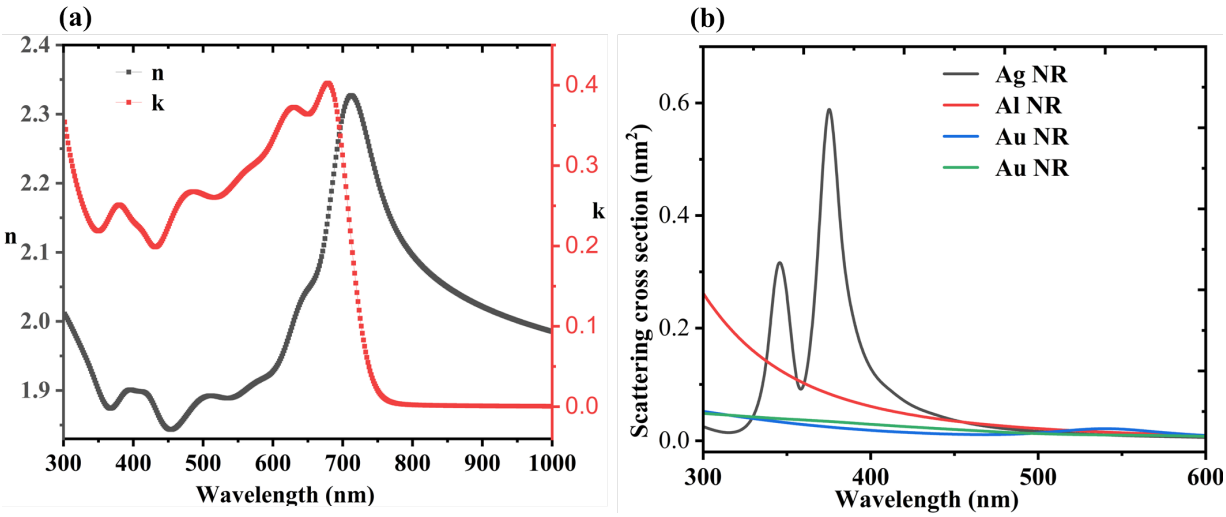

Figure S3: a) real (n) and imaginary (k) refractive indices of the PTB7:$PC_{71}BM$. b) the scattering cross section of PNRs under simulated air (n=1)

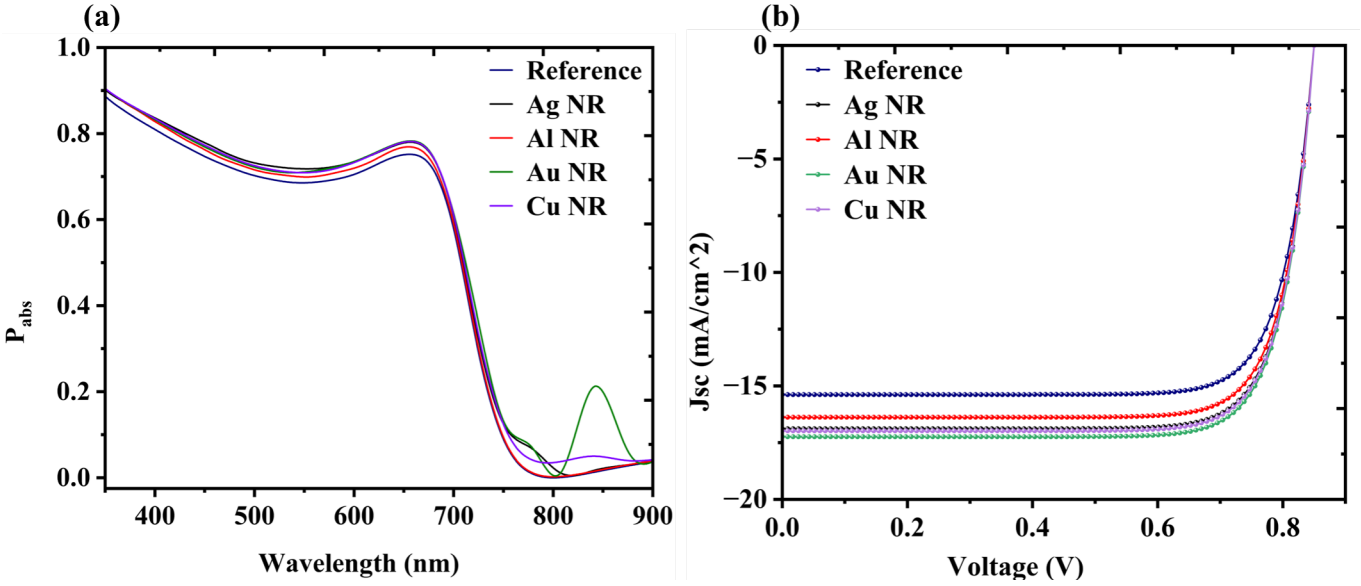

Figure S4: a) The absorption power of PTB7:$PC_{71}BM$ incorporated with Ag, Al, Au, and Cu NRs and b) The J-V curve for four Plasmonic NRs at an optimized AR (1.88)

Table S1: Electrical and optical parameters of active layer, electron transport layers, and hole transport layer of the OSC devices.

Parameters	**PTB7:PC71BM**	**TiO_2**	**MoO_3**
Ionization energy (IE)	5.05	5.85	–
Donor/Acceptor density	0	0	0
Electron affinity (AI)	3.7	3.9	3
Optical band gap (E_{opt})	1.8	1.8	3
Transition band gap (E_t)	2.25	1.90	–
Exciton binding energy (E_{exc})	0.62	0.62	–
Hole mobility (cm^2/Vs)	5.8×10^{-4}	1.3	2.3
Electron mobility (cm^2/Vs)	5×10^{-4}	1.3	–
Absorbance range (nm)	300–750	300–500	–
Relative permittivity	3.9	9	12.5
Energy level (eV)	1.1	–	–
Thickness (nm)	100	–	20
Defect density (cm^{-3})	10^{12}	1×10^{14}	–