Electronic Supplementary Material (ESI) for RSC Advances.

Supplementary Information

Lowering the Work Function PEDOT:PSS by mixing with Barium Acetylacetonate

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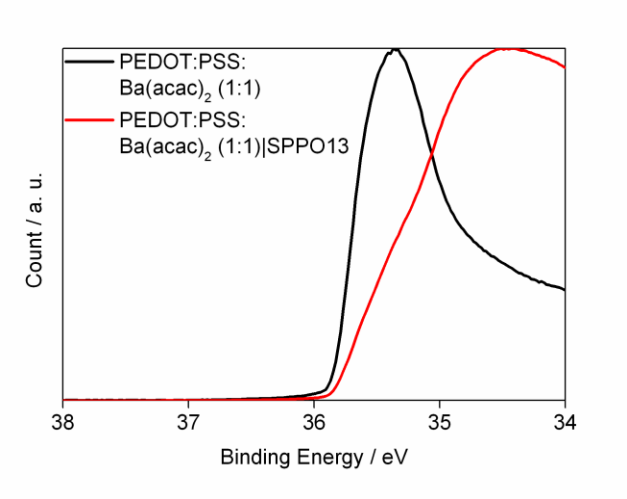
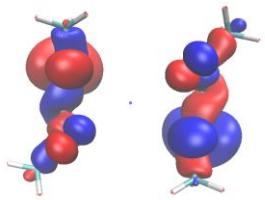
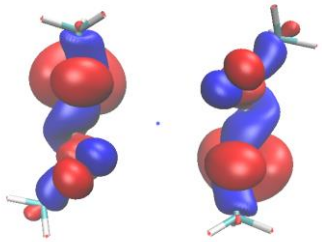
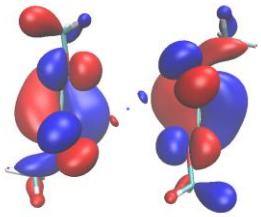
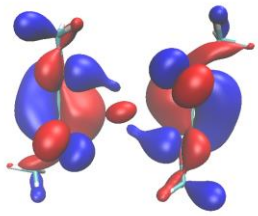
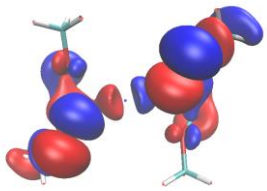
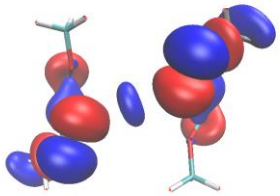
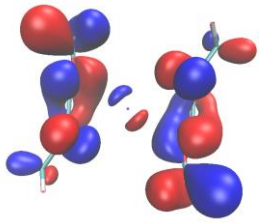
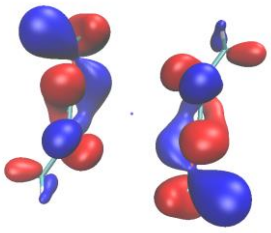
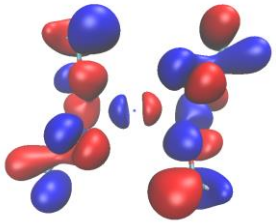
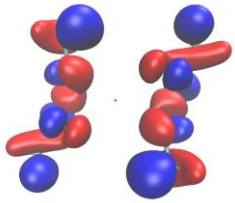
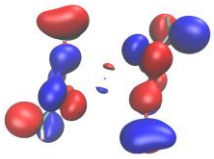
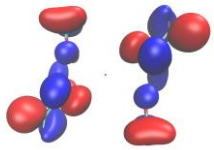
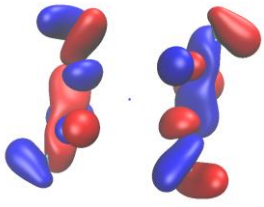
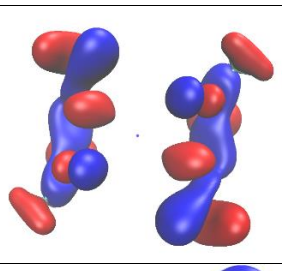
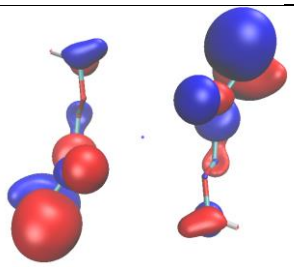
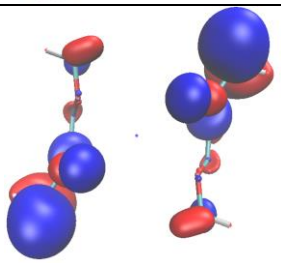
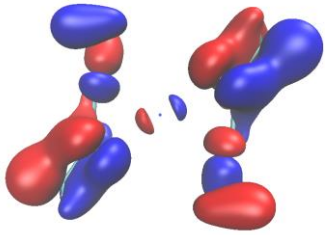
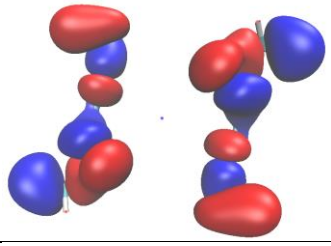
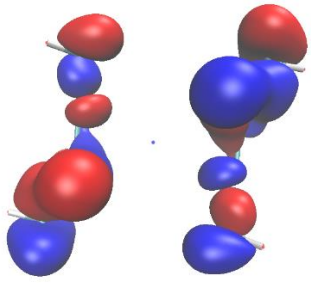
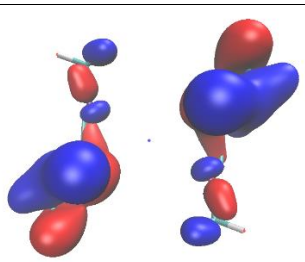
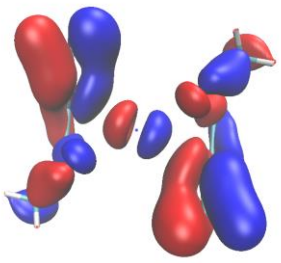
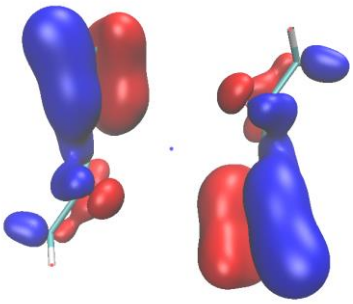
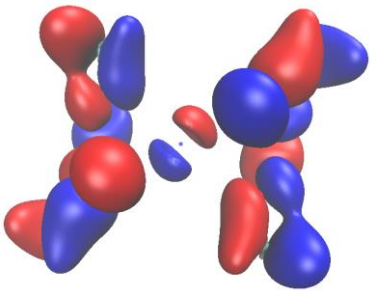
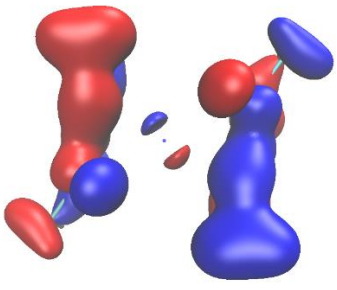


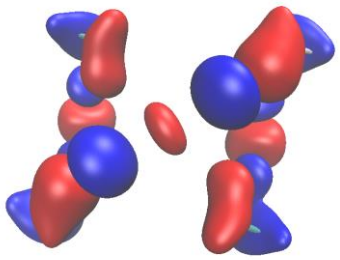
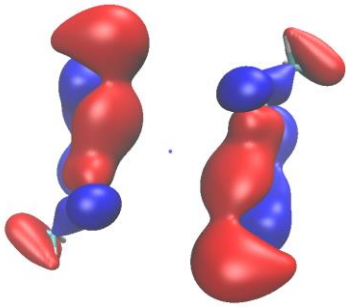
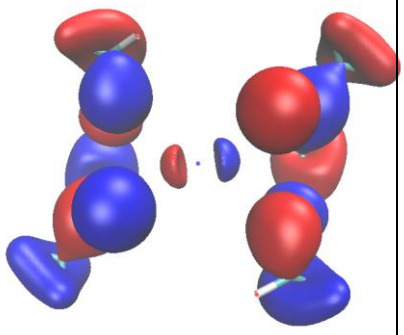
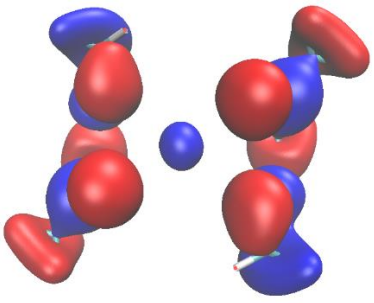
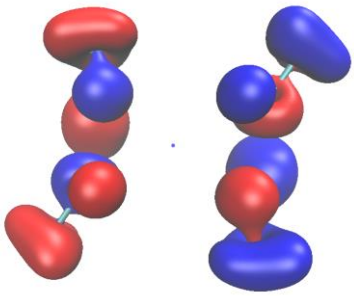
Figure S1: Interfacial dipole between PEDOT:PSS:$Ba(acac)_2$/ SPPO13

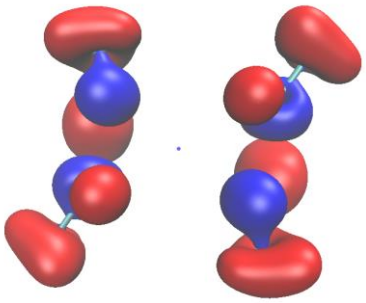
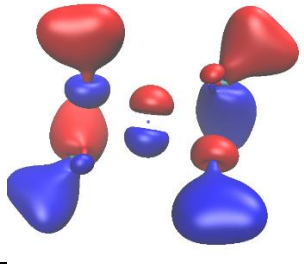
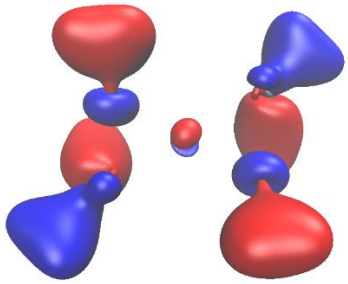
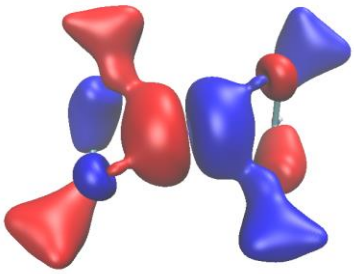
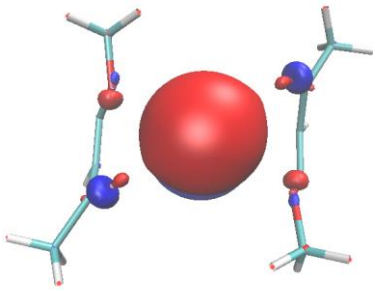
	Energy level (eV)	HOMO levels	Orbital involving barium ions
HOMO	-7.95		
HOMO-1	-7.98		
HOMO-2	-8.56		
HOMO-3	-8.59		x
HOMO-4	-9.71		x
HOMO-5	-9.86		x

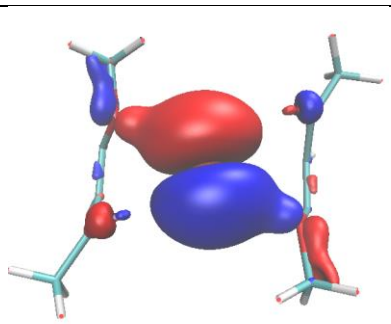
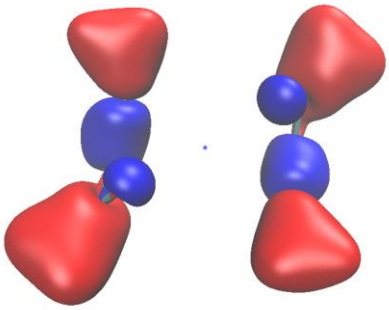
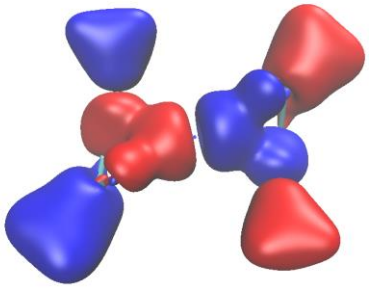
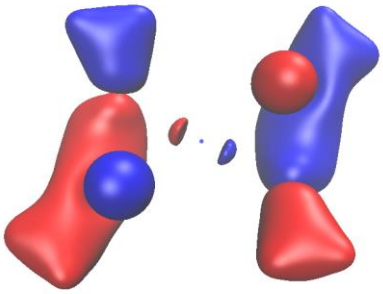
HOMO-6	-11.79		x
HOMO-7	-11.81		
HOMO-8	-12.05		x
HOMO-9	-12.08		
HOMO-10	-12.15		
HOMO-11	-12.19		
HOMO-12	-12.71		

HOMO-13	-12.78		
HOMO-14	-13.29		
HOMO-15	-13.32		
HOMO-16	-13.65		x
HOMO-17	-13.75		
HOMO-18	-14.10		

HOMO-19	-14.12		
HOMO-20	-14.76		x
HOMO-21	-14.80		
HOMO-22	-14.90		x
HOMO-23	-14.95		x

HOMO-24	-15.03		x
HOMO-25	-15.19		
HOMO-26	-16.06		x
HOMO-27	-16.31		x
HOMO-28	-17.98		

HOMO-29	-18.05		
HOMO-30	-21.54		x
HOMO-31	-21.57		x
HOMO-32	-22.15		x
HOMO-33	-22.33		x

HOMO-34	-22.44		x
HOMO-35	-23.12		
HOMO-36	-23.27		x
HOMO-37	-23.76		x

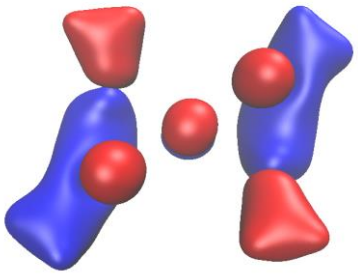
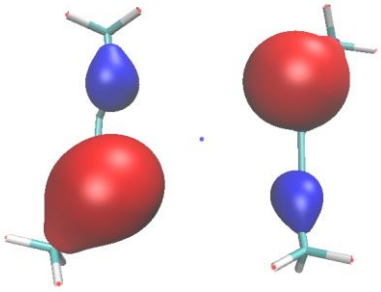
HOMO-38	-23.90		x
HOMO-39	-30.21		

Figure S2: Energy levels and the orbitals of $Ba(acac)_2$ as calculated at unrestricted wB97X functional using def2SVP basis level

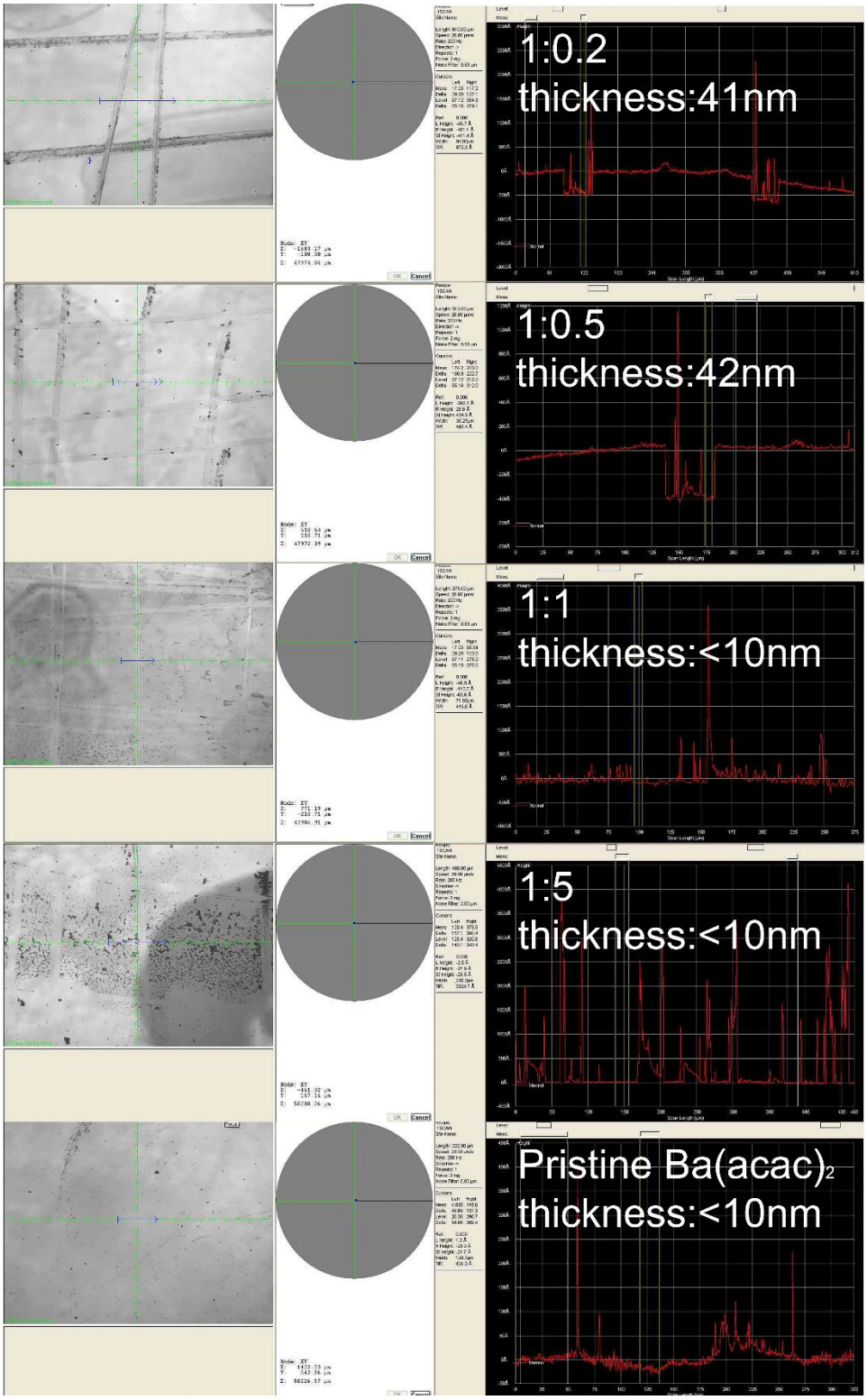
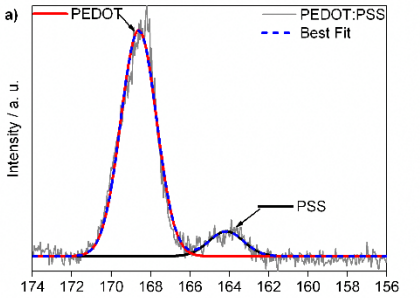
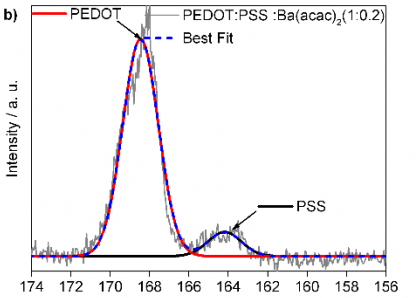


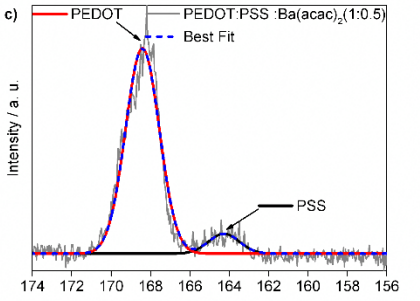
Figure S3: Depth profiling of different films of different concentrations of PEDOT:PSS:$Ba(acac)_2$ (1:X)



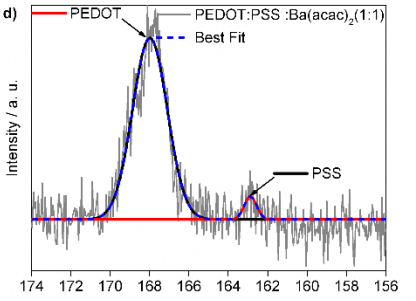
Model	Gaussian	
Equation	y = y0 + A/(w*sqrt(PI/(4*ln(2)))) * exp(-4*ln(2)*(x-xc)^2/w^2)	
Plot	PSS Peak (Count)	PEDOT Peak (Count)
y0	0.05666 ± 0.00238	0.05666 ± 0.00238
xc	164.15236 ± 0.08435	168.60061 ± 0.00941
A	0.20773 ± 0.02022	1.93324 ± 0.02055
w	2.08326 ± 0.21033	2.13544 ± 0.02349
Reduced Chi-Sqr	0.00125	
R-Square(COD)	0.97477	
Adj. R-Square	0.97439	



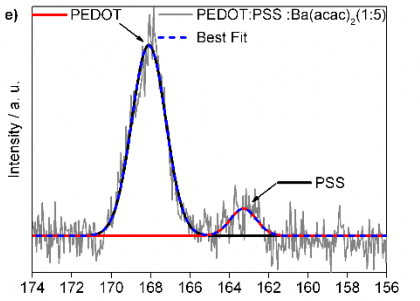
Model	Gaussian	
Equation	y = y0 + A/(w*sqrt(PI/(4*ln(2)))) * exp(-4*ln(2)*(x-xc)^2/w^2)	
Plot	PSS Peak (Count)	PEDOT Peak (Count)
y0	0.05665 ± 0.00276	0.05665 ± 0.00276
xc	164.18186 ± 0.09995	168.45824 ± 0.01149
A	0.19552 ± 0.0231	1.85825 ± 0.024
w	2.01323 ± 0.24844	2.13588 ± 0.02867
Reduced Chi-Sqr	0.00171	
R-Square(COD)	0.96294	
Adj. R-Square	0.96238	



Model	Gaussian	
Equation	y = y0 + A/(w*sqrt(PI/(4*ln(2)))) * exp(-4*ln(2)*(x-xc)^2/w^2)	
Plot	PSS Peak (Count)	PEDOT Peak (Count)
y0	0.06403 ± 0.00253	0.06403 ± 0.00253
xc	164.2677 ± 0.10877	168.41204 ± 0.01105
A	0.14905 ± 0.02049	1.8631 ± 0.02162
w	1.85993 ± 0.26903	2.0218 ± 0.02745
Reduced Chi-Sqr	0.0015	
R-Square(COD)	0.96226	
Adj. R-Square	0.96169	

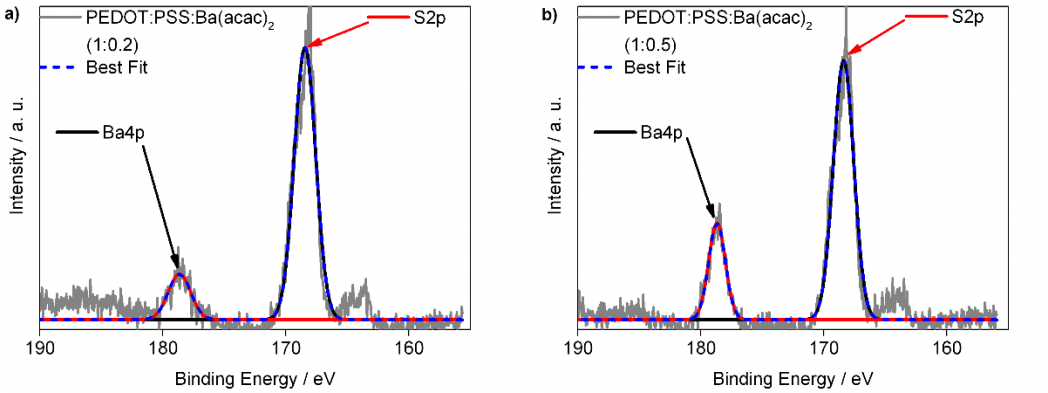


Model	Gaussian	
Equation	y = y0 + A/(w*sqrt(PI/(4*ln(2)))) * exp(-4*ln(2)*(x-xc)^2/w^2)	
Plot	PSS Peak (Count)	PEDOT Peak (Count)
y0	0.19264 ± 0.00433	0.19264 ± 0.00433
xc	162.87503 ± 0.10945	167.98048 ± 0.02338
A	0.06896 ± 0.02196	1.51495 ± 0.04021
w	0.74279 ± 0.26295	2.08182 ± 0.05811
Reduced Chi-Sqr	0.00512	
R-Square(COD)	0.8584	
Adj. R-Square	0.85624	



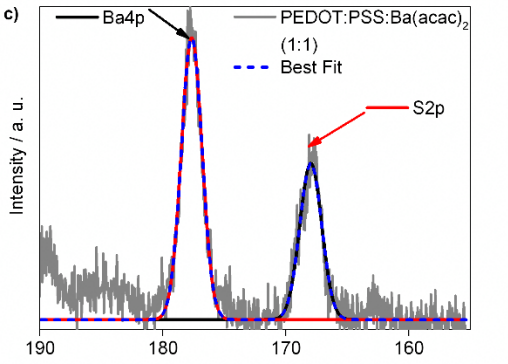
Model	Gaussian	
Equation	y = y0 + A/(w*sqrt(PI/(4*ln(2)))) * exp(-4*ln(2)*(x-xc)^2/w^2)	
Plot	PSS Peak (Count)	PEDOT Peak (Count)
y0	0.13702 ± 0.00392	0.13702 ± 0.00392
xc	163.28072 ± 0.11408	168.08784 ± 0.01862
A	0.1708 ± 0.02892	1.55274 ± 0.0341
w	1.56195 ± 0.28129	2.03217 ± 0.04653
Reduced Chi-Sqr	0.00367	
R-Square(COD)	0.90023	
Adj. R-Square	0.89871	

Figure S4: Curve fitting of S2p peaks of PEDOT:PSS:$Ba(acac)_2$ in order to obtain different ratios of PEDOT to PSS

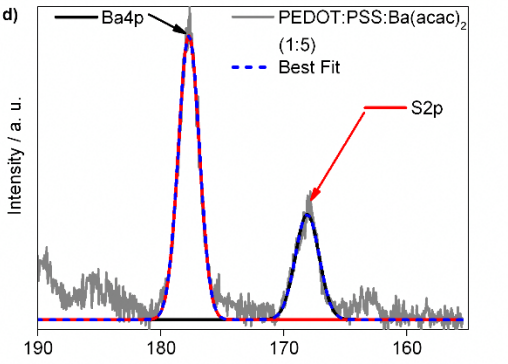


Model	Gauss	
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2)	
Plot	S2p (Count)	Ba4p (Count)
y0	0.03 ± 0	0.03 ± 0
xc	168.44449 ± 0.01273	178.65341 ± 0.07784
w	1.73724 ± 0.02545	1.8232 ± 0.15567
A	1.83557 ± 0.02329	0.32263 ± 0.02386
Reduced Chi-Sqr	0.00235	
R-Square(COD)	0.92021	
Adj. R-Square	0.91964	

Model	Gauss	
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2)	
Plot	S2p (Count)	Ba4p (Count)
y0	0.03 ± 0	0.03 ± 0
xc	168.3986 ± 0.0107	178.6877 ± 0.02597
w	1.6613 ± 0.02141	1.35766 ± 0.05194
A	1.67076 ± 0.01864	0.5087 ± 0.01685
Reduced Chi-Sqr	0.00157	
R-Square(COD)	0.94297	
Adj. R-Square	0.94256	



Model	Gauss	
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2)	
Plot	S2p (Count)	Ba4p (Count)
y0	0.03 ± 0	0.03 ± 0
xc	167.97679 ± 0.03485	177.66121 ± 0.01875
w	1.78234 ± 0.0697	1.67701 ± 0.03747
A	1.08165 ± 0.03663	1.83483 ± 0.03552
Reduced Chi-Sqr	0.00566	
R-Square(COD)	0.84033	
Adj. R-Square	0.83918	



Model	Gauss	
Equation	y=y0 + (A/(w*sqrt(PI/2)))*exp(-2*((x-xc)/w)^2)	
Plot	S2p (Count)	Ba4p (Count)
y0	0.03 ± 0	0.03 ± 0
xc	168.0988 ± 0.04358	177.72966 ± 0.01516
w	1.93192 ± 0.08715	1.70001 ± 0.03029
A	0.78908 ± 0.03083	1.8716 ± 0.0289
Reduced Chi-Sqr	0.0037	
R-Square(COD)	0.87609	
Adj. R-Square	0.8752	

e)

	PEDOT:PSS:Ba(acac) (1:X)			
	1:0.2	1:0.5	1:1	1:5
S2p Peak Area	1.83	1.67	1.08	0.79
Ba3d Peak Area	0.32	0.51	1.83	1.87
S2p Peak Area Corrected*	3.4	3.09	2	1.46
Ba3d Peak Area Corrected*	0.14	0.22	0.78	0.8
Elemental Ratio of Sulphur/Barium	25	14	2.6	1.8

*Corrected with Photoionization Cross-section

Figure S5: Integration of area of S2p to Ba 4p by curve fitting of the films in order to obtain different ratios of Ba and S.

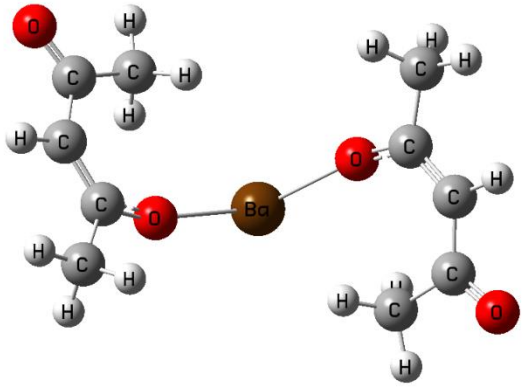


Figure S6: Optimized structure of $Ba(acac)_2$ using unrestricted wB97X functional using def2-QZVP basis level

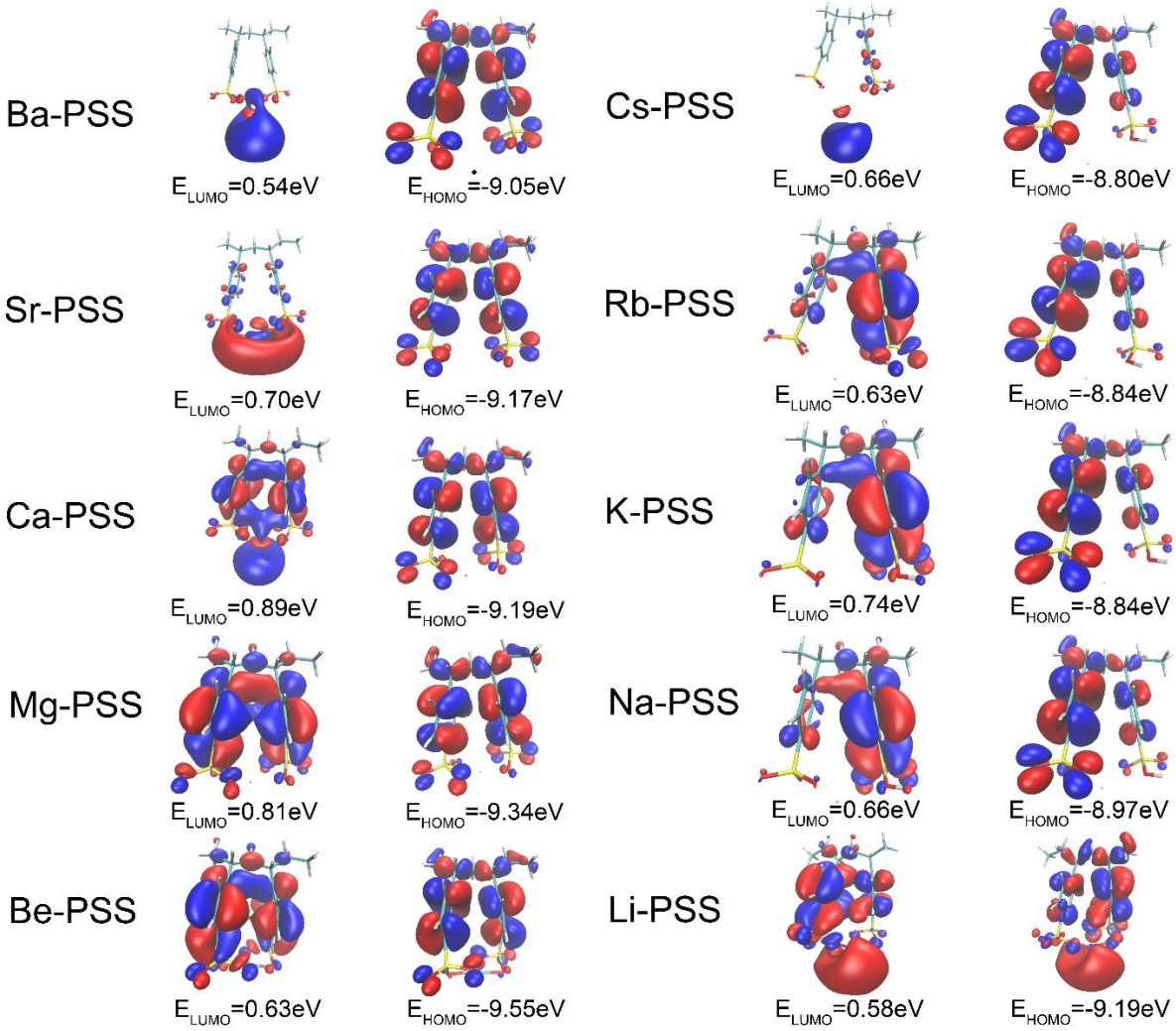


Figure S7: Frontier orbitals of M-PSS where M is the alkaline metal from group 1 or 2 and their energy levels optimized using unrestricted wB97X functional using def2SVP basis level.

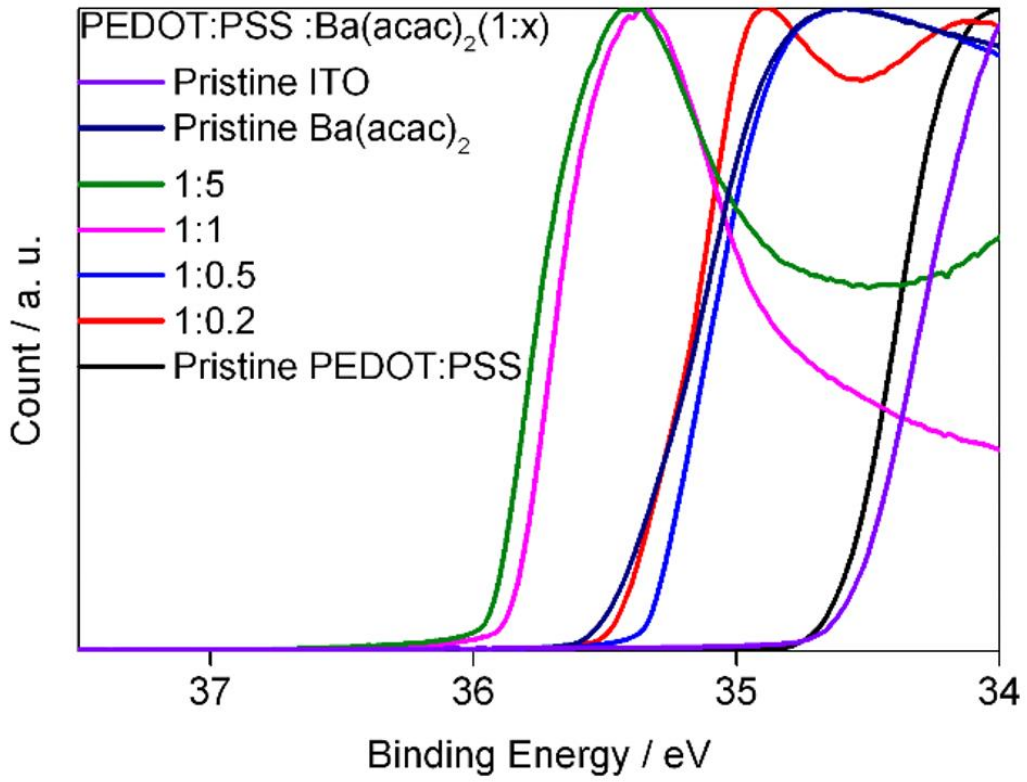


Figure S8 High energy cut off onset from the UPS spectra for PEDOT:PSS , ITO and PEDOT:PSS:$Ba(acac)_2$ at different ratios

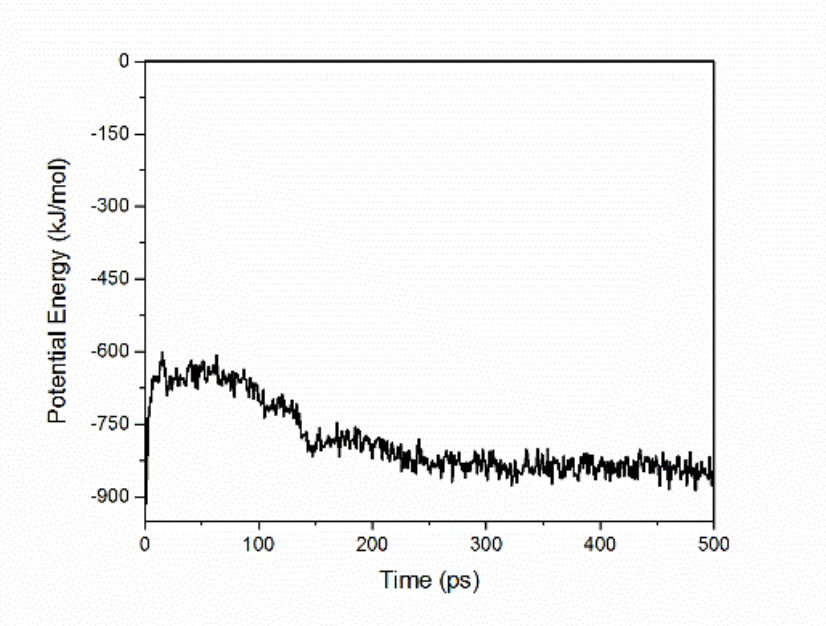


Figure S9: The potential energy of molecular dynamic simulations for PEDOT: PSS: $Ba(acac)_2$ for the duration of 500 ps

Table S1: The interaction energy between PEDOT:PSS with/without $Ba(acac)_2$

System	Energy (CHARMM) kcal/mol))			
	PEDOT: PSS	**PEDOT**	**PSS**	**Interaction Energy**
PEDOT: PSS	4343.47	1229.56	3033.57	80.34
PEDOT: PSS: $Ba(acac)_2$	3028.33	656.71	2256.62	115.00

Table 2: Molecular coordinate of $Ba(acac)_2$ optimized using unrestricted wB97X functional using def2-QZVP basis level

O	-4.047375349	3.03434598	0.644328456
C	-3.358384951	2.094835125	0.290860638
C	-2.214562294	2.381395324	-0.678916298
C	-3.602181748	0.752597432	0.777256739
C	-2.959280315	-0.406926826	0.461176133
O	-1.972611123	-0.522726035	-0.37857735
C	-3.385158054	-1.700318667	1.100507401
O	1.8512618	0.41105193	-0.378903274
C	2.85490809	0.400200178	0.448443547
C	3.139971028	1.727843221	1.094800794
C	3.627133895	-0.683523661	0.74468742
C	3.527927305	-2.037778957	0.241622952
C	2.42631997	-2.431067143	-0.740054707
Ba	-0.036715144	-0.144025194	-1.622151041
H	-2.237533195	3.43527891	-0.940208849
H	-2.337911248	1.778902176	-1.582495114
H	-1.259745012	2.155585514	-0.195937175
H	-4.416587139	0.695232594	1.484752056
H	-4.196285656	-1.567968468	1.810911397
H	-2.531275367	-2.146162741	1.612156603
H	-3.698672938	-2.40042094	0.324863668
H	3.964822776	1.680590583	1.800214724
H	2.245642895	2.075491309	1.613111369
H	3.372252708	2.462754507	0.32271145
H	4.435351227	-0.54494168	1.447990279
H	2.566120343	-3.47130816	-1.019015256
H	2.480516226	-1.801378462	-1.631318832
H	1.451482834	-2.322976247	-0.255899724
O	4.310626567	-2.904505162	0.586005102