Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

π-π Interactions Effect on Single-molecule Electron Transport Properties of tetraphenylethene molecule and its derivatives: A First-Principles Study

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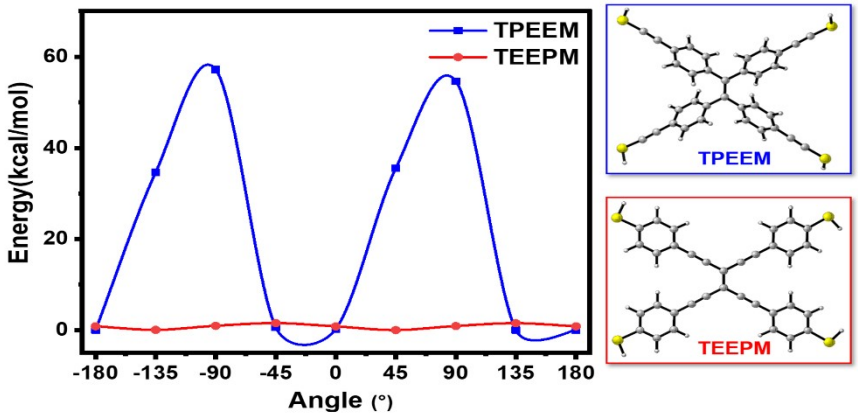

Figure S1. The energy barriers of phenyls rotation in the TMEPE and TMPEE molecules.

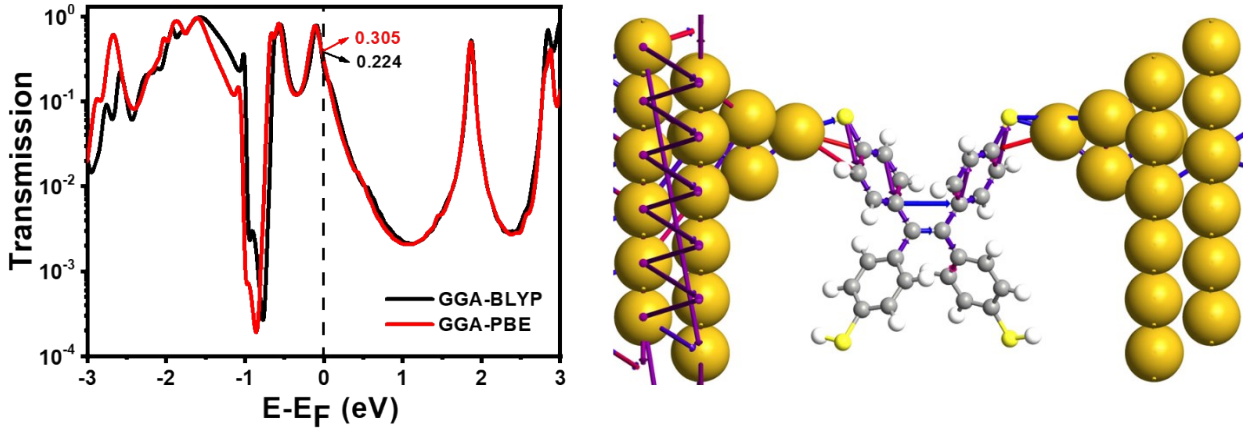

Figure S2. (a) The calculated electron transmission spectra of the Au/TPEM-cis/Au molecular junction under the GGA-PBE and GGA-BLYP methods and (b) the fitted transmission pathway of the Au/TPEM-cis/Au molecular junction by the GGA-BLYP method.

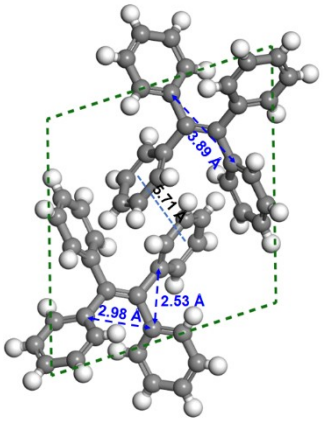

Figure S3. The molecular crystal structure of TPE molecule (CCDC 156130), and the distances between molecules were selectively annotated.

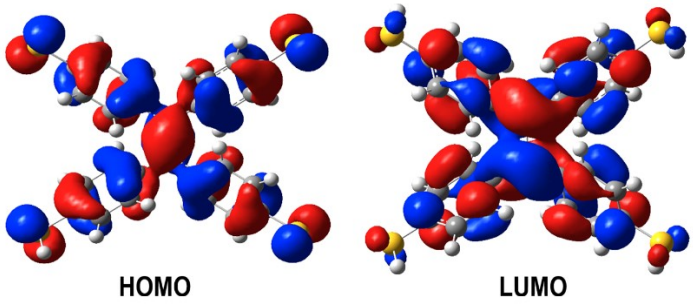

Figure S4. The calculated HOMO and LUMO of TPEM molecule.

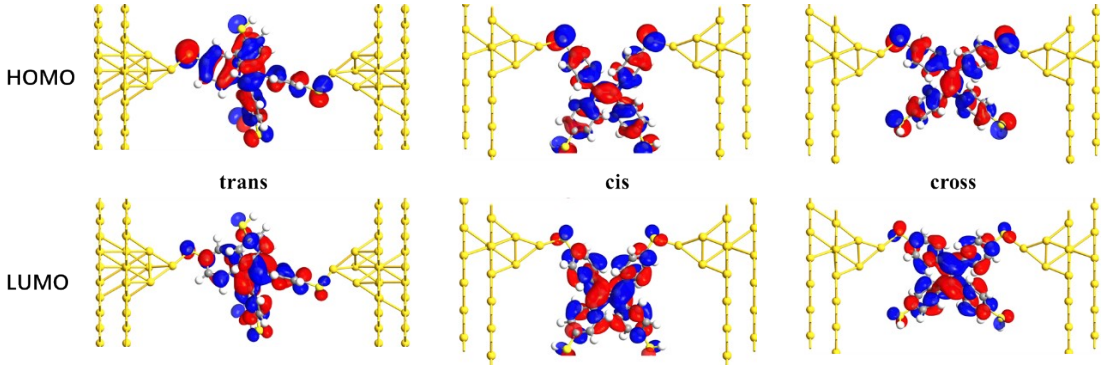

Figure S5. MPSH of the TPEM molecular junction at zero bias.

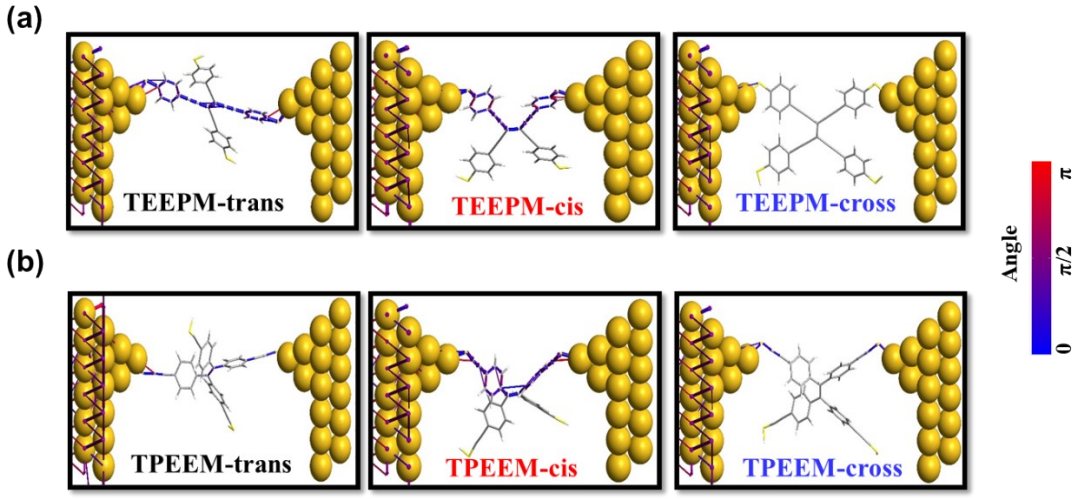

Figure S6. The transmission pathways of TEEPM (a) and TPEEM (b) molecules with three different π-conjugated structures.

Table S1. Molecular coordinates for TPEM molecule.

TPEM	x	y	Z		x	y	z
C	-0.00136000	-0.68356900	0.00073300	C	2.64885700	-3.36220200	-0.54286700
C	-0.00259400	0.68587100	-0.00017200	C	0.78239800	-2.84631200	-1.45762000
C	-1.25170000	1.48963100	0.14761600	C	3.33494800	-1.97871800	1.31289600

C	-2.19411200	1.20964500	1.15216400	C	2.01531000	-0.37355600	1.82821700
C	-1.49906800	2.59567400	-0.68308000	C	3.58028100	-3.06247400	0.45883600
C	-3.33908400	1.98284800	1.30886800	C	2.81540400	-4.19965700	-1.21431600
H	-2.02255600	0.37494500	1.82334900	C	4.03767600	-1.74085100	2.10609400
C	-2.64822800	3.36867000	-0.54337200	C	1.24593500	1.49047700	-0.14892500
H	-0.78147100	2.85161000	-1.45654500	C	1.49675900	2.59434800	0.68511400
C	-3.58141700	3.06877600	0.45665900	C	2.18530200	1.21188500	-1.15537400
H	-4.04347800	1.74460100	2.10044800	C	2.64780200	3.36278600	0.54668900
H	-2.81229800	4.20782800	-1.21325200	C	0.78171900	2.84759100	1.46173000
C	-1.24918200	-1.48944700	-0.14755200	C	3.33230200	1.98399000	-1.31318200
C	-2.18937900	-1.21362200	-1.15527400	C	2.01153000	0.37900700	-1.82840800
C	-1.49740300	-2.59318100	0.68596600	C	3.57930000	2.11953758	-0.68603924
C	-3.33314000	-1.98861100	-1.31249100	C	2.82192500	2.92724215	-3.62731017
H	-2.01747400	-0.38009900	-1.82786900	C	4.03071800	2.17103439	-4.28381688
C	-2.64506000	-3.36827800	0.54536500	C	-5.07478800	3.47334424	-2.69447196
H	-0.78179700	-2.84539800	1.46251700	C	-4.85732200	3.51598275	-4.52231338
C	-3.57612400	-3.07247600	-0.45788500	C	5.02462600	-2.94310030	-0.28559022
H	-4.03653500	-1.75272700	-2.10567800	C	5.64574800	-1.97778986	-0.00770659
H	-2.80971100	-4.20578000	1.21719000	C	5.07588800	-2.84219431	0.37896412
C	1.24838400	-1.48653100	0.14954000	C	4.85823100	-3.14960391	-0.93057856
C	1.49850700	-2.59086800	-0.68259100	C	-5.06646600	0.54814542	-0.00133582
C	2.18892000	-1.20697200	1.15595000	C	-4.86284900	-4.91033200	0.28095800

Table S2. Molecular coordinates for TEEPM molecule

TEEPM	x	y	z		x	y	z
C	0.00001700	-0.69982800	-0.69982800	H	4.67826700	-5.97042500	-0.28643000
C	0.00003100	0.69986300	0.69986300	C	-3.45481000	-2.81381400	-0.16065100
C	-1.21078300	1.43229600	1.43229600	C	-3.48366300	-4.19606200	0.11241200
C	1.21131300	1.43201900	1.43201900	C	-4.66481100	-2.17638200	-0.50653800
C	1.21129200	-1.43199900	-1.43199900	C	-4.67274200	-4.91145800	0.04670500
C	-1.21080000	-1.43225800	-1.43225800	H	-2.56214500	-4.70271600	0.37921700
C	-2.24188500	2.07925900	2.07925900	C	-5.85265700	-2.89105900	-0.57304700
C	2.24231800	2.07922400	2.07922400	H	-4.65768100	-1.11469100	-0.73031500
C	2.24228400	-2.07922100	-2.07922100	C	-5.86962900	-4.26657700	-0.29586800
C	-2.24189700	-2.07923400	-2.07923400	H	-4.66665100	-5.97552200	0.26329100
C	3.45528300	2.81366900	2.81366900	H	-6.77206800	-2.38038100	-0.84341700
C	4.66067000	2.17902000	2.17902000	C	-3.45478200	2.81386200	0.16057500
C	3.48810000	4.19411000	4.19411000	C	-3.48360700	4.19615700	-0.11217300
C	5.84992800	2.89336200	2.89336200	C	-4.66482000	2.17634200	0.50623400
H	4.65080100	1.11933300	1.11933300	C	-4.67269800	4.91154700	-0.04638300
C	4.67634500	4.90796700	4.90796700	H	-2.56208500	4.70289000	-0.37881300
H	2.56942200	4.69862000	4.69862000	C	-5.85265100	2.89101100	0.57284200
C	5.87031000	4.26532600	4.26532600	H	-4.65769400	1.11459700	0.72974500
H	6.76364600	2.37999900	2.37999900	C	-5.86959800	4.26661100	0.29598100

H	4.67819300	5.97051500	5.97051500	H	-4.66658900	5.97565700	-0.26275300
C	3.45524000	-2.81367900	-2.81367900	H	-6.77210600	2.38030500	0.84301400
C	4.66053400	-2.17911800	-2.17911800	S	7.35686100	5.24833100	-0.36780800
C	3.48812600	-4.19405600	-4.19405600	H	8.18352300	4.26463800	- 0.77152600
C	5.84978300	-2.89348000	-2.89348000	S	-7.43361200	5.11711900	0.40036000
H	4.65062300	-1.11948600	0.74976800	H	-6.97696400	6.33839300	0.06293900
C	4.67634700	-4.90792900	-0.06206400	S	-7.43363100	-5.11711000	-0.40010600
H	2.56951100	-4.69848500	-0.41417600	H	-6.97694900	-6.33830700	-0.06248400
C	5.87022800	-4.26537200	0.29951600	S	7.35677700	-5.24838500	0.36804100
H	6.76342900	-2.38017100	0.87278800	H	8.18329100	-4.26478700	0.77229500

Table S3. Molecular coordinates for TPEPM molecule.

TPEPM	x	y	z		x	y	z
C	0.00022600	0.68444600	0.00013800	C	-3.58397700	3.06785700	0.46072900
C	0.00073400	-0.68582900	-0.00036600	H	-2.82055600	4.20226500	-1.20997700
C	1.24952000	-1.48875700	0.14798100	H	-4.03876700	1.74512200	2.10521100
C	2.18735500	-1.20857700	1.15799400	C	-1.24740000	-1.48967500	-0.14920700
C	1.49782200	-2.59262100	-0.68865400	C	-1.49340900	-2.59584200	0.68511700
C	3.33182200	-1.97915700	1.31539100	C	-2.18665800	-1.20781200	-1.15753700
H	2.00984900	-0.37560600	1.82971500	C	-2.64158100	-3.36481000	0.54648100
C	2.64467900	-3.36316200	-0.54825700	H	-0.77558800	-2.84652300	1.45988000
H	0.78091700	-2.84265200	-1.46450500	C	-3.32867700	-1.98141800	-1.31753600
C	3.58504600	-3.06932700	0.45923600	H	-2.01033100	-0.37336900	-1.82771800
H	4.03862700	-1.74853100	2.10559400	C	-3.58151500	-3.07189800	-0.46161100
H	2.82293600	-4.20166400	-1.21345200	H	-2.82098700	-4.20203600	1.21297500
C	1.24845200	1.48824600	-0.14816000	H	-4.03452700	-1.75270200	-2.10914600
C	2.18691900	1.20831000	-1.15766200	C	-4.75488800	-3.86358200	-0.61777900
C	1.49540000	2.59286300	0.68788000	C	-5.74669500	-4.55677500	-0.74199100
C	3.33070000	1.97988000	-1.31513100	C	4.75846000	-3.86062500	0.61516300
H	2.01043200	0.37478200	-1.82895800	C	5.75542500	-4.54778700	0.73088000
C	2.64161000	3.36435600	0.54746400	C	4.75531000	3.86311200	-0.61552100
H	0.77791700	2.84276400	1.46322700	C	5.75163200	4.55119700	-0.73130100
C	3.58260400	3.07079100	-0.45952200	C	-4.75750700	3.85898100	0.61657600
H	4.03799100	1.74946700	-2.10496300	C	-5.75456800	4.54605400	0.73200100
H	2.81881800	4.20344200	1.21219800	S	-7.20202500	-5.38746100	-1.00223300
C	-1.24840300	1.48747800	0.14911400	H	-6.89133600	-6.52124800	-0.33269900
C	-1.49595200	2.59248900	-0.68624800	S	7.18585300	-5.40868700	1.02813300
C	-2.18688800	1.20618000	1.15821800	H	7.08116300	-6.29656100	0.01302200
C	-2.64284400	3.36291600	-0.54570900	S	7.18128300	5.41342100	1.02841300
H	-0.77846600	2.84343300	-1.46125500	H	7.07501200	6.30200000	0.01408300
C	-3.33140300	1.97667200	1.31578100	S	-7.18521500	5.40678000	1.02863400
H	-2.00993100	0.37239700	1.82908200	H	-7.07959600	6.29533400	0.01421100