Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supplementary Information for:

Exploring structure based charge transport relationships in phenyl diketopyrrolopyrrole single crystals using a 2D π-π dimer model system

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SI.1 CSD identifier, monomer dihedral angle, measured intermonomer displacements, stacking axis, intermolecular interactions and charge transfer integrals for π-π dimer pairs of reported PDPP crystal structures

Table SI.1.1 CSD identifier, monomer dihedral angle (θ), measured intermonomer displacements (Δx/y/z), stacking axis, intermolecular interactions (ΔE_{CP}) and hole/electron transfer integrals ($t_{h/e}$) for π-π dimer pairs of reported **PDPP** crystal structures. [a] kJ mol^{-1}

CSD identifier	θ / °	Δ(x/y/z) / Å	Stacking axis	ΔE_{CP} [a]	t_h/t_e [a]
EBIGUR04[1]	51.41	0.59/5.26/3.14	a	-58.90	1.10/2.86
EKUFAT[2]	44.14/39.40	1.34/1.18/3.92	b	-74.42	5.01/5.19
EKUFEX[2]	50.71	7.82/0.41/3.88	a	-52.25	2.69/3.71
EREHAM[3]	30.43	9.13/1.64/3.35	b	-41.08	0.27/0.79
	30.43	0.58/4.43/2.78	a	-56.17	3.47/5.12
FOVYAS[4]	22.23/2.94	3.40/1.01/3.31	a	-62.24	5.23/7.11
GATJIX[5]	32.35/29.90	3.57/0.23/3.42	b	-79.16	1.96/7.50
GAJTOD[5]	29.44/34.59	3.55/0.05/3.66	b	-79.36	2.17/4.54
GEGHUX[6]	26.23	9.42/0.15/3.71	c	-77.80	8.60/4.58
GEGJAF[6]	23.72	9.17/0.15/3.78	c	-100.16*	11.52/2.13*
GEGJEJ[6]	24.85	9.14/0.17/3.72	c	-140.89*	6.86/1.80*
GORLOQ[7]	29.24	3.45/0.30/3.37	b	-155.81	0.80/9.63
HEJCEG[8]	40.49	9.07/1.20/3.34	a	-96.55	3.97/4.11
HEJCOQ[8]	41.88	9.13/0.90/3.54	a	-61.19	0.12/0.73
HOZNER[9]	20.56	8.44/0.05/3.37	a	-39.46	1.02/5.09
HUTLEO[10]	26.11	8.44/0.47/3.78	b	-51.52	3.60/3.02
HUYZUW[11]	63.27	5.03/1.26/5.02	a	-51.09	1.71/0.08
KAWMUR[12]	42.30	1.06/1.90/5.33	b	-36.39	0.57/0.05
KAWNAY[12]	24.68/2.74	3.34/2.32/4.06	b	-66.67	5.07/6.93
LAHCIJ[13]	12.70	3.48/0.51/3.45	b	-103.45	5.54/15.11
MUNHEK[14]	0.69	3.46/3.09/3.26	-	-47.84	2.49/4.01
	0.69	2.37/4.35/3.15	-	-37.06	11.62/2.93
OKUZUQ[15]	21.28	8.26/1.21/3.66	b	-42.48	4.35/9.26
PAMYUY[16]	3.11/8.69	5.01/0.10/3.34	a	-68.82	14.58/4.82
QOHGAX[9]	22.49	4.52/0.05/3.44	a	-70.12	10.69/6.13
QOHGEB[9]	22.12	9.40/0.31/3.32	c	-35.52	6.03/1.41
QUYHIC[17]	33.02	3.28/1.80/4.10	a	-60.73	1.87/1.79
SAPDES[18]	14.44	1.82/5.52/2.92	a	-14.48	2.41/1.20
	14.44	0.68/1.51/3.27	b	-57.15	4.64/4.51
UKATOR[19]	38.23	3.72/0.35/3.90	a	-71.02	0.50/3.68
UKATUX[19]	30.43	9.12/2.31/3.59	b	-22.46	2.01/0.89

VARKII01[20]	48.35	1.28/1.47/4.08	a	-63.06	5.03/4.48
WEBKAP[21]	9.73	1.03/1.80/3.34	a	-67.45	9.48/1.87
WEBKET[21]	2.39	3.40/3.13/3.32	c	-48.11	1.75/2.27
	2.39	2.25/4.58/3.23	a	-36.13	9.51/3.11
WEPCUQ[22]	5.58	0.44/1.66/3.53	b	-43.39	2.72/4.97
WOHDAY[23]	10.72	0.91/1.53/3.36	c	-54.83	8.34/2.47
WUTCEU[24]	44.03	9.39/1.22/3.22	b	-42.51	4.38/1.67
WUTCEU01[9]	20.07	5.13/0.28/3.38	c	-69.60	11.77/3.96
WUTCEU02[9]	43.97	9.39/1.22/3.22	b	-42.51	4.38/1.67
XATKIN[25]	43.06	8.61/0.98/3.16	-	-58.64	0.44/3.80

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SI.2 Chemical structures and space-filled representation for π-π dimer pairs of reported PDPP crystal structures

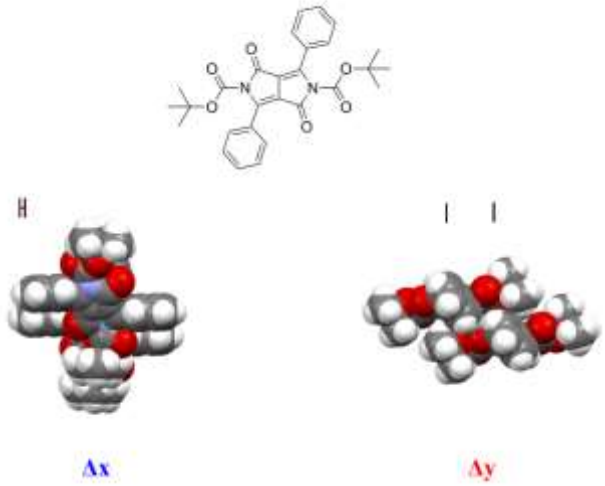

Figure SI.2.1 Chemical structure and space-filled illustration of π-π dimer pair of **EBIGUR04**

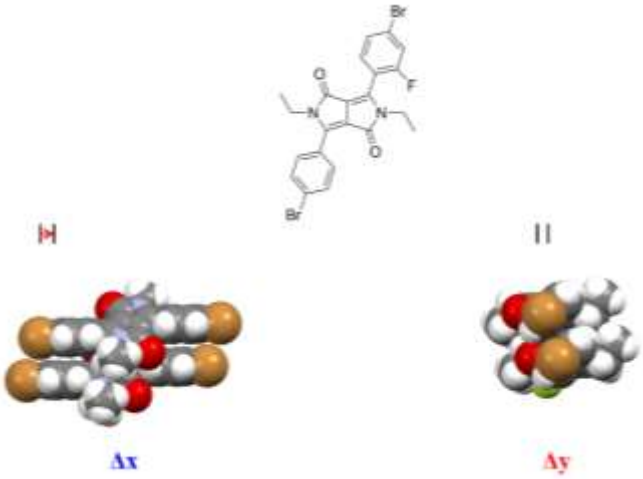

Figure SI.2.2 Chemical structure and space-filled illustration of π-π dimer pair of **EKUFAT**

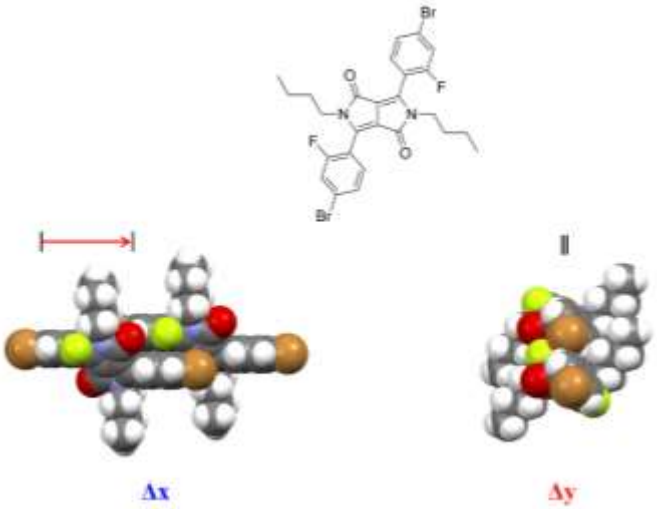

Figure SI.2.3 Chemical structure and space-filled illustration of π-π dimer pair of **EKUFEX**

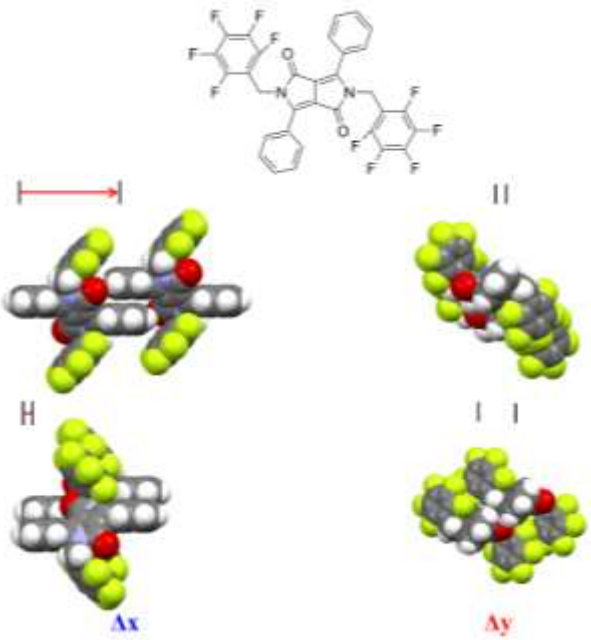

Figure SI.2.4 Chemical structure and space-filled illustration of π-π dimer pair of **EREHAM**

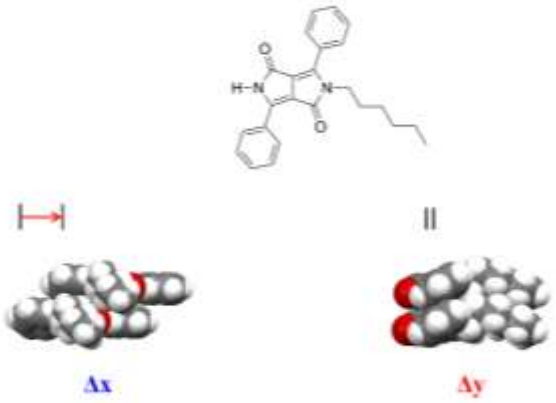

Figure SI.2.5 Chemical structure and space-filled illustration of π-π dimer pair of **FOVYAS**

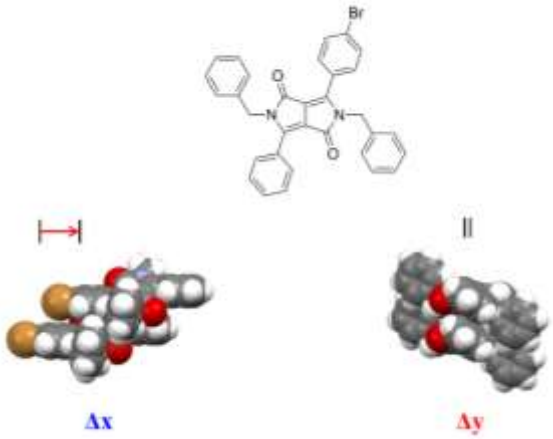

Figure SI.2.6 Chemical structure and space-filled illustration of π-π dimer pair of **GATJIX**

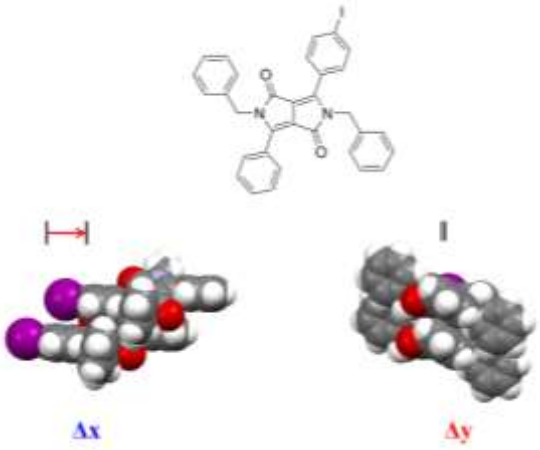

Figure SI.2.7 Chemical structure and space-filled illustration of π-π dimer pair of **GAJTOD**

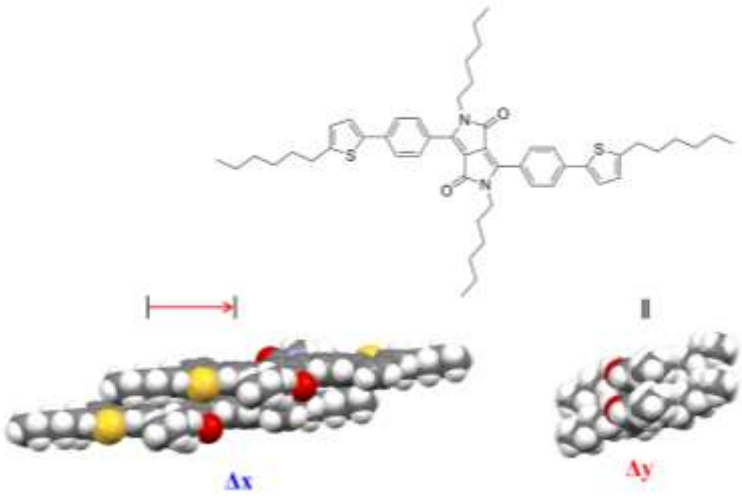

Figure SI.2.8 Chemical structure and space-filled illustration of π-π dimer pair of **GEGHUX**

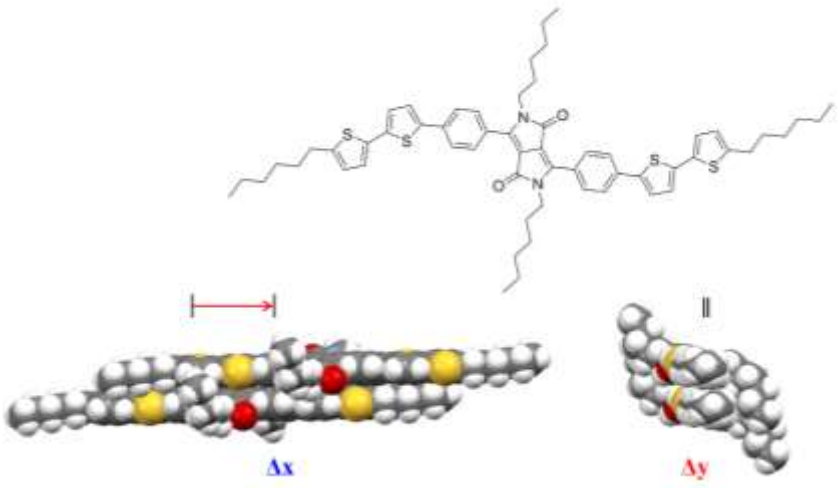

Figure SI.2.9 Chemical structure and space-filled illustration of π-π dimer pair of **GEGJAF**

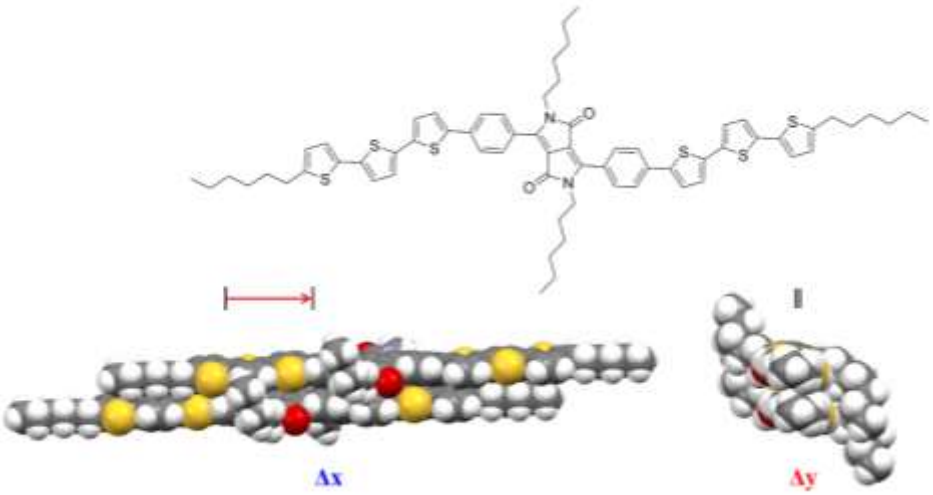

Figure SI.2.10 Chemical structure and space-filled illustration of π-π dimer pair of **GEGJEJ**

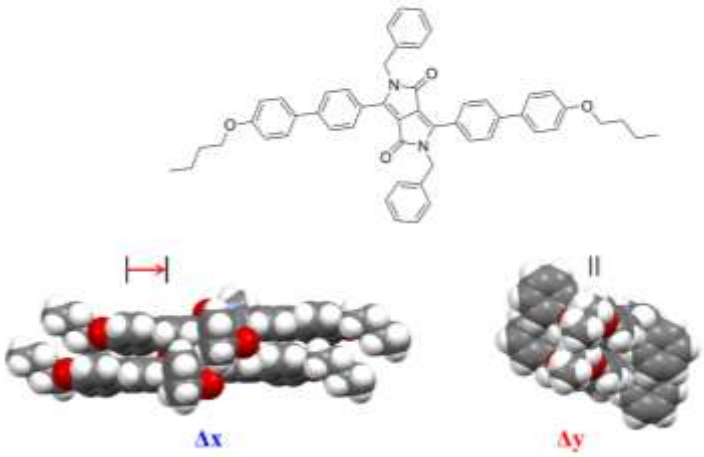

Figure SI.2.11 Chemical structure and space-filled illustration of π-π dimer pair of **GORLOQ**

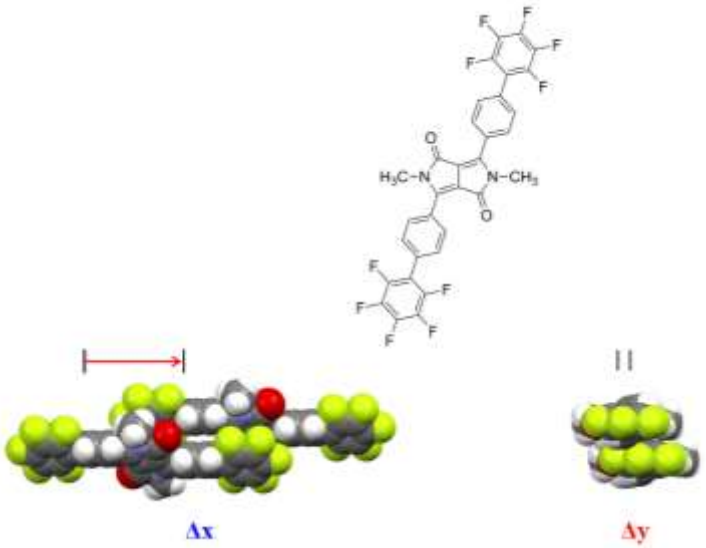

Figure SI.2.12 Chemical structure and space-filled illustration of π-π dimer pair of **HEJCEG**

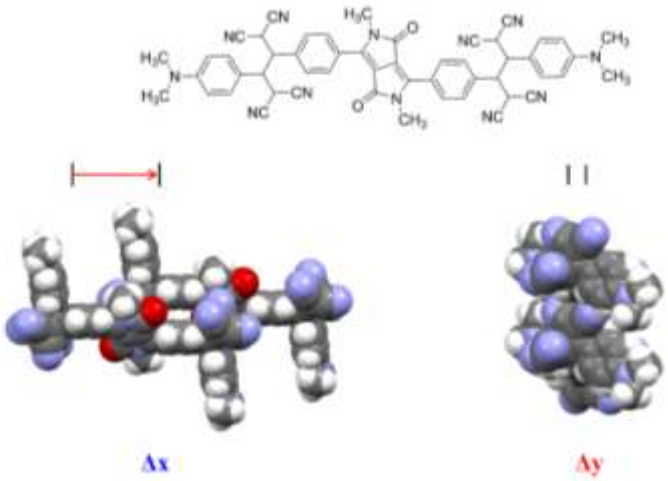

Figure SI.2.13 Chemical structure and space-filled illustration of π-π dimer pair of **HEJCOQ**

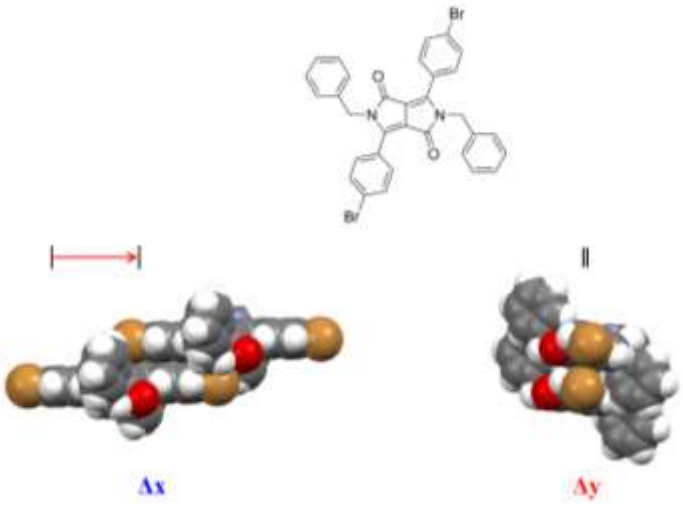

Figure SI.2.14 Chemical structure and space-filled illustration of π-π dimer pair of **HOZNER**

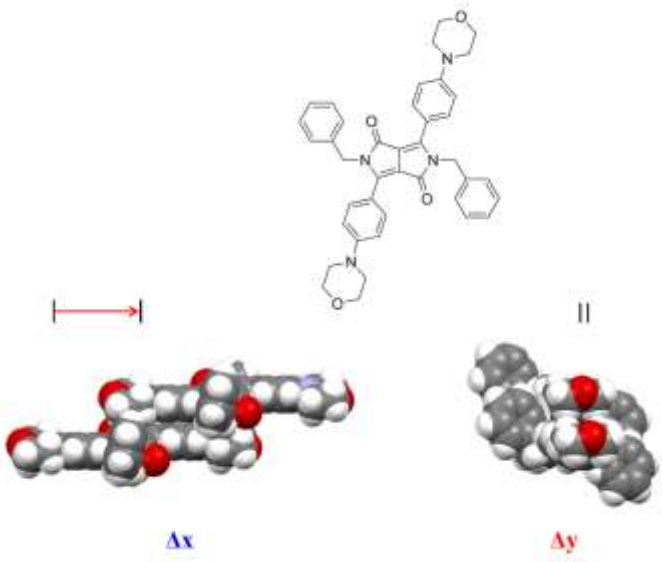

Figure SI.2.15 Chemical structure and space-filled illustration of π-π dimer pair of **HUTLEO**

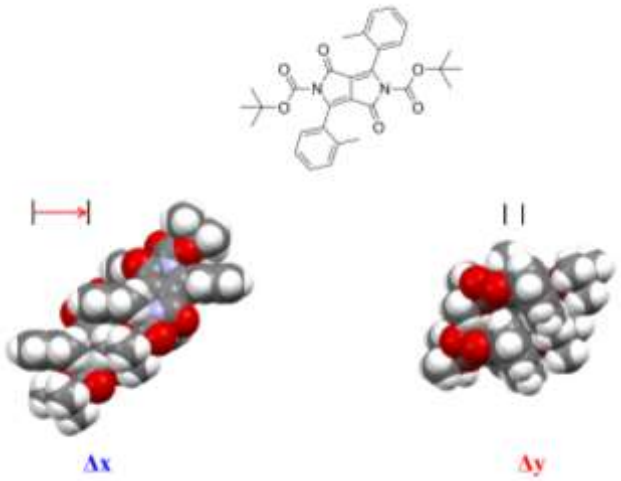

Figure SI.2.16 Chemical structure and space-filled illustration of π-π dimer pair of **HUYZUW**

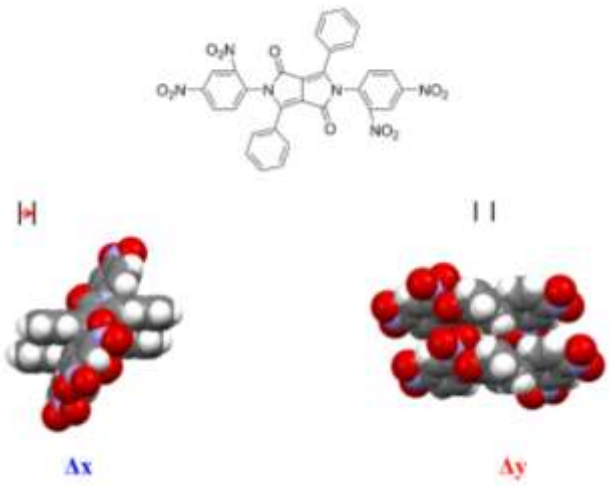

Figure SI.2.17 Chemical structure and space-filled illustration of π-π dimer pair of **KAWMUR**

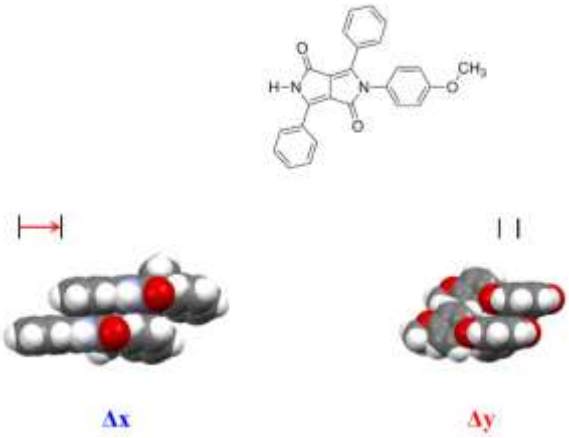

Figure SI.2.18 Chemical structure and space-filled illustration of π-π dimer pair of **KAWNAY**

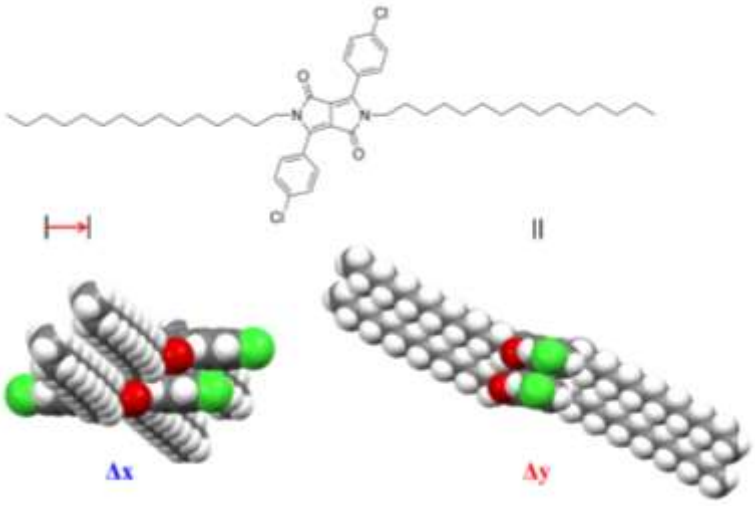

Figure SI.2.19 Chemical structure and space-filled illustration of π-π dimer pair of **LAHCIJ**

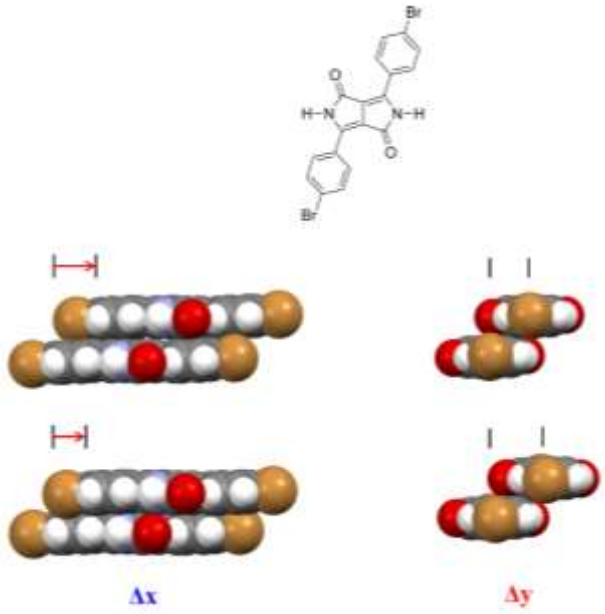

Figure SI.2.20 Chemical structure and space-filled illustration of π-π dimer pair of **MUNHEK**

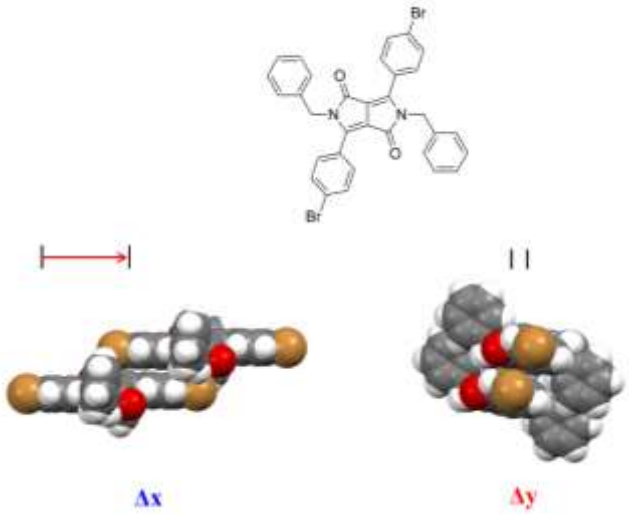

Figure SI.2.21 Chemical structure and space-filled illustration of π-π dimer pair of **OKUZUQ**

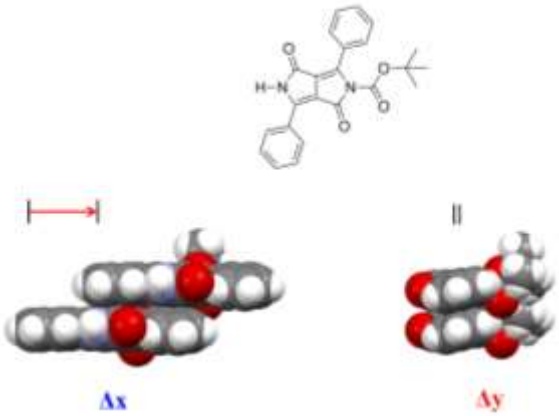

Figure SI.2.22 Chemical structure and space-filled illustration of π-π dimer pair of **PAMYUY**

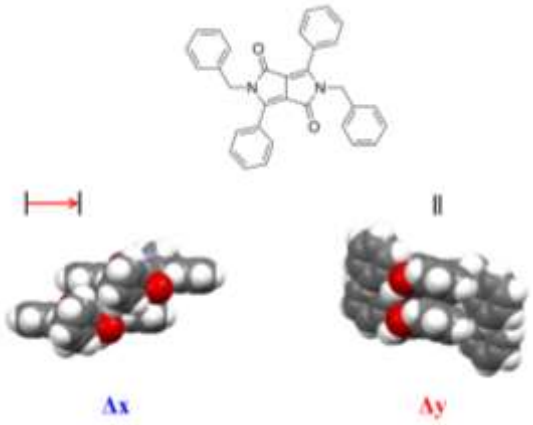

Figure SI.2.23 Chemical structure and space-filled illustration of π-π dimer pair of **QOHGAX**

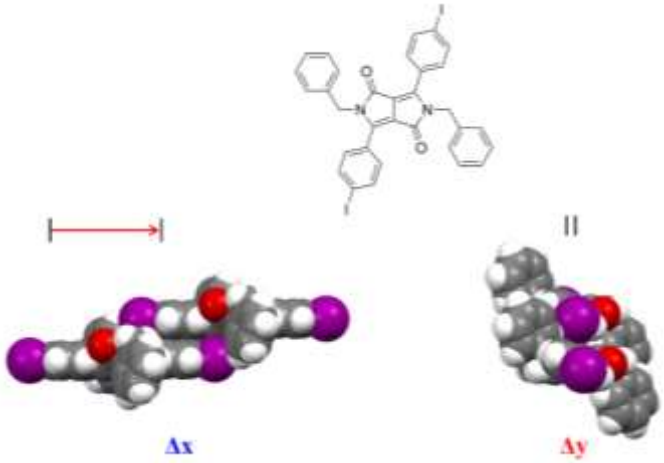

Figure SI.2.24 Chemical structure and space-filled illustration of π-π dimer pair of **QOHGEB**

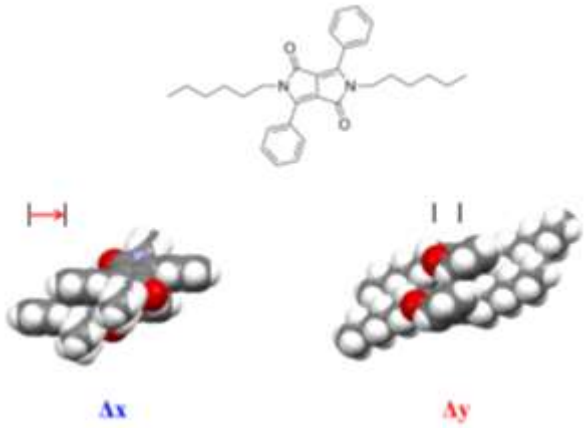

Figure SI.2.25 Chemical structure and space-filled illustration of π-π dimer pair of **QUYHIC**

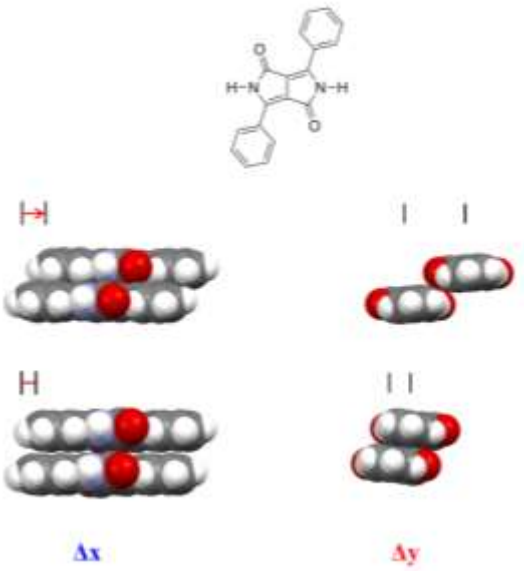

Figure SI.2.26 Chemical structure and space-filled illustration of π-π dimer pair of **SAPDES**

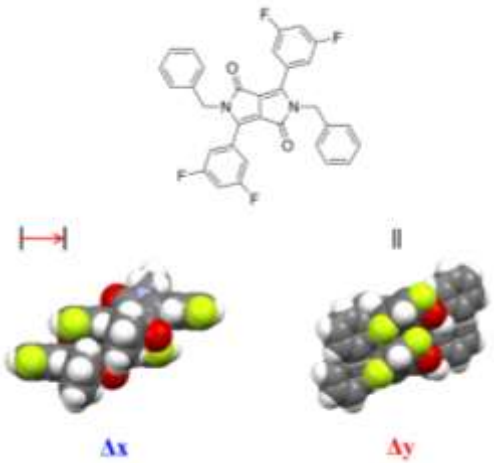

Figure SI.2.27 Chemical structure and space-filled illustration of π-π dimer pair of **UKATOR**

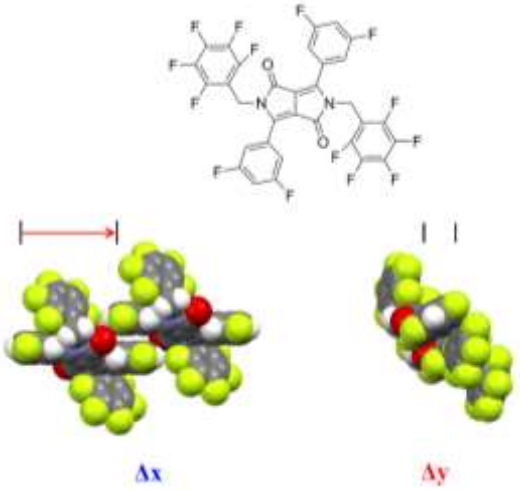

Figure SI.2.28 Chemical structure and space-filled illustration of π-π dimer pair of **UKATUX**

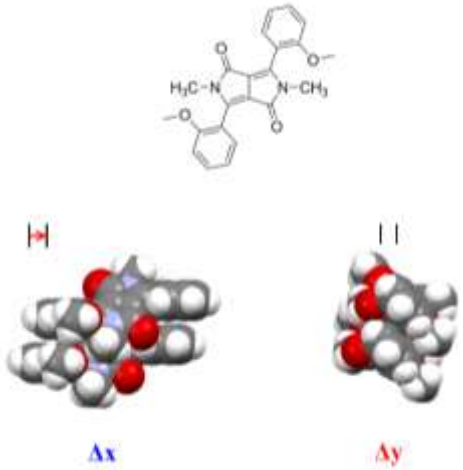

Figure SI.2.29 Chemical structure and space-filled illustration of π-π dimer pair of **VARKII01**

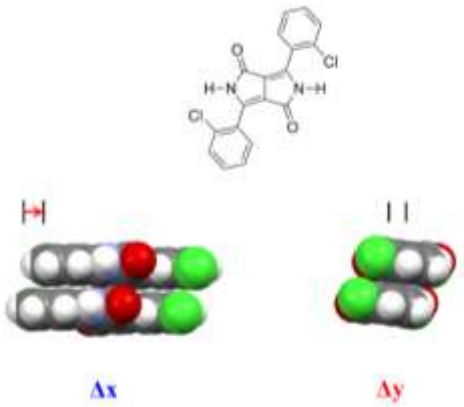

Figure SI.2.30 Chemical structure and space-filled illustration of π-π dimer pair of **WEBKAP**

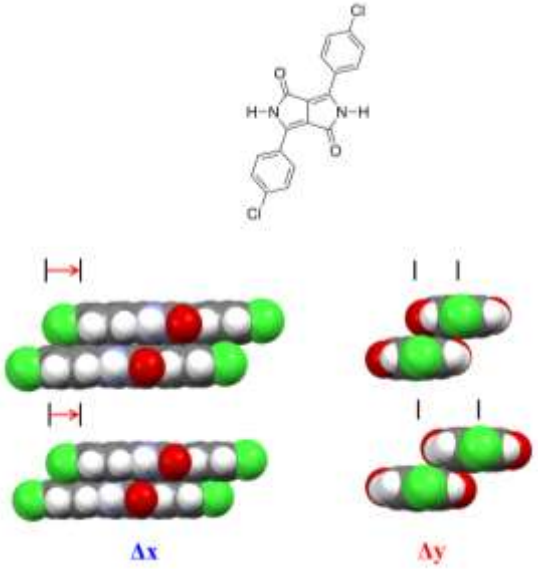

Figure SI.2.31 Chemical structure and space-filled illustration of π-π dimer pair of **WEBKET**

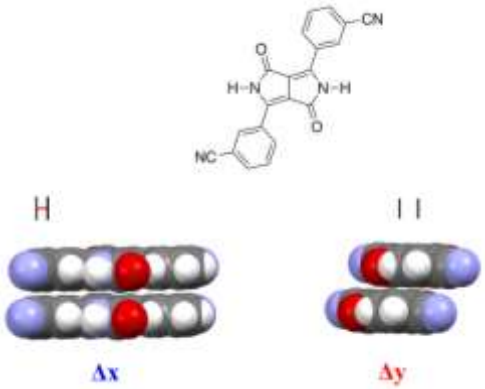

Figure SI.2.32 Chemical structure and space-filled illustration of π-π dimer pair of **WEPCUQ**

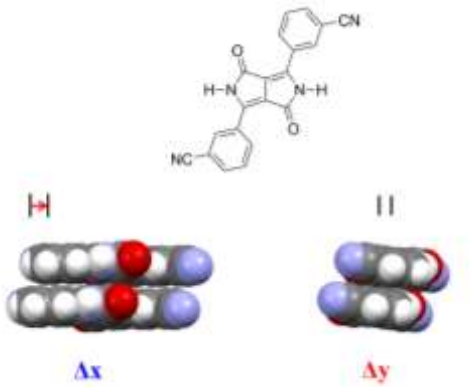

Figure SI.2.33 Chemical structure and space-filled illustration of π-π dimer pair of **WOHDAY**

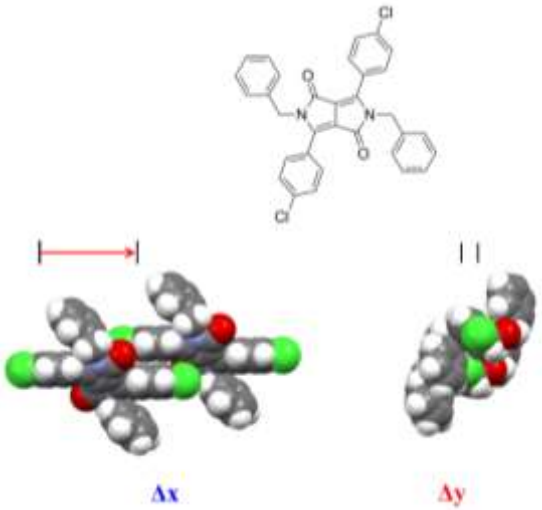

Figure SI.2.34 Chemical structure and space-filled illustration of π-π dimer pair of **WUTCEU**

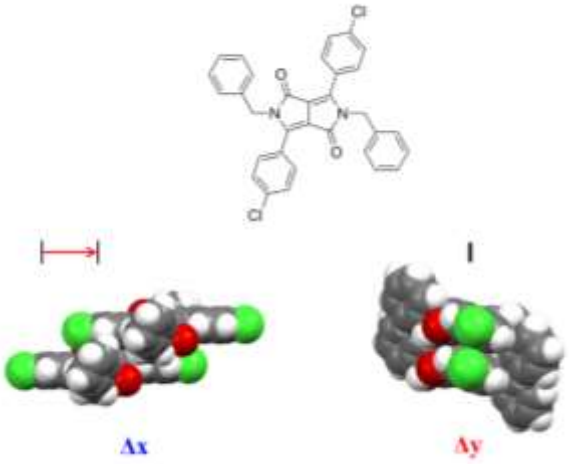

Figure SI.2.35 Chemical structure and space-filled illustration of π-π dimer pair of **WUTCEU01**

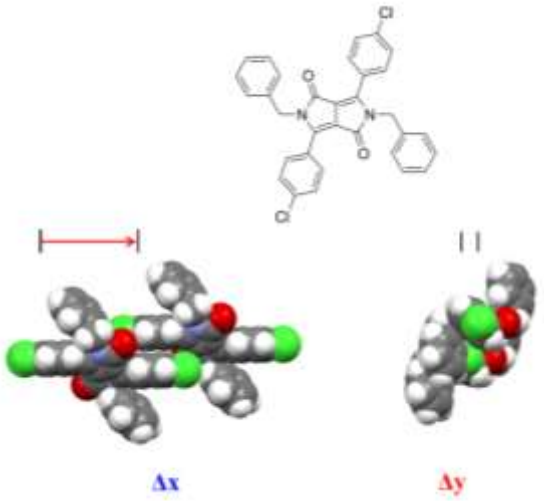

Figure SI.2.36 Chemical structure and space-filled illustration of π-π dimer pair of **WUTCEU02**

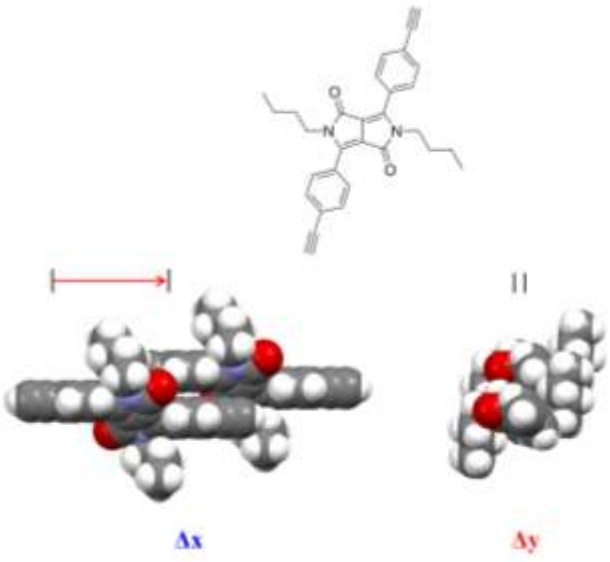

Figure SI.2.37 Chemical structure and space-filled illustration of π-π dimer pair of **XATKIN**

SI.3 Geometry of optimised PDPP monomer employed in dimer model system

Atom	x / Å	y / Å	z / Å
N	-0.130	-0.784	0.999
C	-0.669	0.493	1.000
C	0.385	1.372	1.000
C	1.615	0.628	1.000
C	1.281	-0.797	1.000
H	-0.648	-1.647	1.001
C	0.719	2.797	1.000
C	2.669	1.507	1.000
N	2.130	2.784	1.001
H	2.648	3.647	0.999
C	-2.108	0.731	1.000
C	-4.857	1.237	1.000
C	-2.586	2.049	1.000
C	-3.027	-0.326	1.001
C	-4.390	-0.074	1.001
C	-3.951	2.293	1.000
H	-1.884	2.876	1.000
H	-2.692	-1.357	1.002
H	-5.089	-0.902	1.001
H	-4.309	3.316	0.999
H	-5.923	1.433	1.000
C	4.108	1.269	1.000
C	6.857	0.763	1.000
C	5.027	2.326	0.999
C	4.586	-0.049	1.000
C	5.951	-0.293	1.000
C	6.390	2.074	0.999
H	4.692	3.357	0.998
H	3.884	-0.876	1.000
H	6.309	-1.316	1.001
H	7.089	2.902	0.999
H	7.923	0.567	1.000
O	0.061	3.812	1.000
O	1.939	-1.812	1.000

SI.4 Computed intermolecular interactions and charge transfer integrals for key dimer pairs employing ωB97X-D density functional

Table SI.4.1. Intermolecular interactions (ΔE_{CP}) and charge transfer integrals (t_h/t_e) for selected **PDPP** based systems using wB97X-D and M06-2X density functionals at 6-311G(d) level.

PDPP system	**ΔE_{CP} / kJ mol^{-1}**		**$t_{h/e}$ / kJ mol^{-1}**	
	M06-2X	**wB97X-D**	**M06-2X**	**wB97X-D**
Model dimer (0.0,0.0,3.6) Å	-24.64	-49.77	26.2/28.94	25.45/26.86
Model dimer (3.3,0.3,3.6) Å	-54.69	-72.93	7.78/5.03	7.91/5.15
Model dimer (5.1,2.1,3.6) Å	-35.95	-50.40	3.39/2.33	3.45/1.88
Model dimer (7.2,3.0,3.6) Å	-24.26	-34.82	0.31/3.62	0.22/3.36
Model dimer (9.0,3.9,3.6) Å	-11.52	-16.95	0.42/1.07	0.42/1.07
Model dimer (11.1,5.1,3.6) Å	-3.25	-4.52	0.09/0.08	0.09/0.07
SAPDES	-57.16	-73.78	4.64/5.51	4.62/4.33
	-14.48	-24.84	2.41/1.20	2.56/1.31
HOZNER	-39.46	-62.21	1.02/5.09	0.80/4.73
KAWNAY	-66.67	-93.67	5.07/6.93	5.13/6.56
QOHGAX	-70.12	-108.66	10.69/6.13	11.00/5.25
WEBKAP	-67.45	-83.63	9.48/1.87	9.37/1.78
EREHAM	-41.08	-58.22	0.27/0.79	0.36/0.86