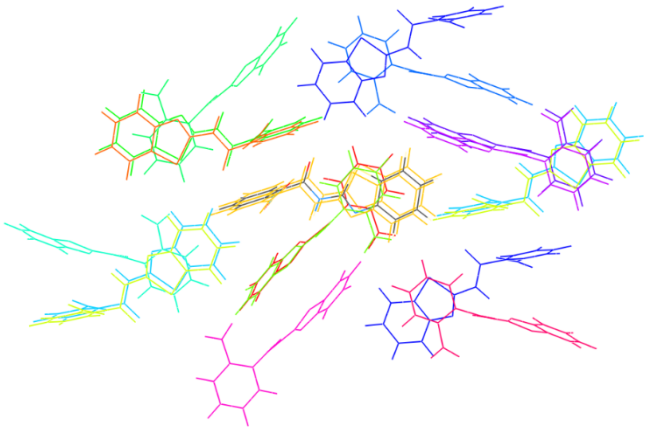
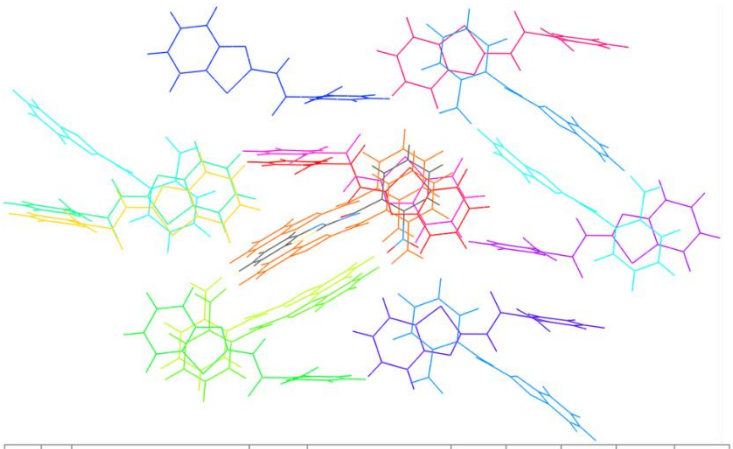
Supplementary Materials:



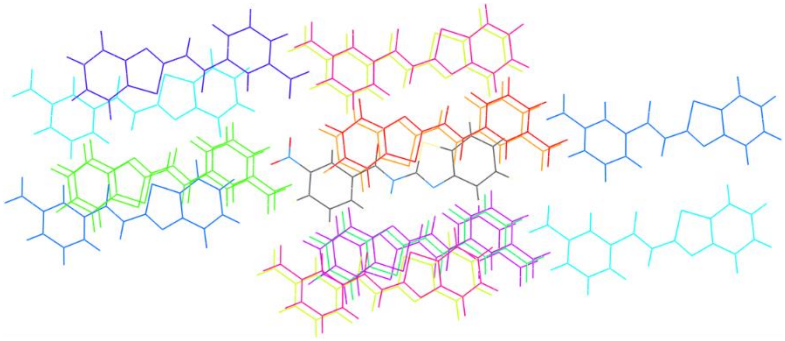
	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-	3.70	B3LYP/6-31G(d,p)	-80.6	-18.6	-86.6	123.7	-97.9
	1	-x, -y, -z	9.71	B3LYP/6-31G(d,p)	-16.7	-3.8	-17.2	13.4	-27.2
	2	x, y, z	7.61	B3LYP/6-31G(d,p)	-8.4	-2.3	-10.7	13.1	-11.8
	2	-x+1/2, y+1/2, -z+1/2	12.59	B3LYP/6-31G(d,p)	-3.4	-1.2	-11.8	7.9	-9.9
	1	-	5.63	B3LYP/6-31G(d,p)	-14.0	-4.8	-44.7	25.5	-41.5
	1	-x, -y, -z	6.95	B3LYP/6-31G(d,p)	-18.0	-6.2	-42.1	26.0	-44.2
	1	-	8.60	B3LYP/6-31G(d,p)	5.8	-1.4	-8.8	2.7	-0.9
	1	-	12.70	B3LYP/6-31G(d,p)	-2.3	-1.4	-6.9	3.2	-7.5
	2	-x+1/2, y+1/2, -z+1/2	12.90	B3LYP/6-31G(d,p)	-5.4	-1.4	-10.2	10.4	-9.2
	1	-	8.82	B3LYP/6-31G(d,p)	-7.1	-2.1	-9.6	11.3	-10.4
	2	x+1/2, -y+1/2, z+1/2	10.45	B3LYP/6-31G(d,p)	-3.7	-1.2	-6.2	3.5	-8.0
	1	-	11.31	B3LYP/6-31G(d,p)	-0.7	-0.3	-11.6	6.3	-7.2
	1	-	12.65	B3LYP/6-31G(d,p)	0.3	-0.1	-5.8	2.5	-3.3
	1	-	8.79	B3LYP/6-31G(d,p)	-5.5	-1.2	-10.2	6.5	-11.6
	1	-	12.29	B3LYP/6-31G(d,p)	-1.9	-0.6	-5.9	1.8	-6.5

Figure S1. Interaction energies for a 3.8 Å cluster around IA.



	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-	3.70	B3LYP/6-31G(d,p)	-80.6	-18.6	-86.6	123.7	-97.9
	2	x, y, z	7.61	B3LYP/6-31G(d,p)	3.4	-1.7	-10.8	6.6	-3.0
	1	-	12.65	B3LYP/6-31G(d,p)	0.3	-0.1	-5.8	2.5	-3.3
	1	-x, -y, -z	6.52	B3LYP/6-31G(d,p)	-9.3	-3.0	-24.5	24.3	-18.4
	1	-x, -y, -z	7.81	B3LYP/6-31G(d,p)	-10.4	-2.1	-56.8	45.9	-33.6
	1	-	8.79	B3LYP/6-31G(d,p)	-5.5	-1.2	-10.2	6.5	-11.6
	1	-	11.31	B3LYP/6-31G(d,p)	-0.7	-0.3	-11.6	6.3	-7.2
	2	-x+1/2, y+1/2, -z+1/2	12.17	B3LYP/6-31G(d,p)	-5.1	-1.4	-10.0	12.7	-7.2
	2	x+1/2, -y+1/2, z+1/2	11.40	B3LYP/6-31G(d,p)	-7.1	-1.2	-4.0	2.8	-10.1
	1	-	8.60	B3LYP/6-31G(d,p)	5.8	-1.4	-8.8	2.7	-0.9
	1	-	8.82	B3LYP/6-31G(d,p)	-7.1	-2.1	-9.6	11.3	-10.4
	1	-	12.70	B3LYP/6-31G(d,p)	-2.3	-1.4	-6.9	3.2	-7.5
	1	-	5.63	B3LYP/6-31G(d,p)	-14.0	-4.8	-44.7	25.5	-41.5
	1	-	12.29	B3LYP/6-31G(d,p)	-1.9	-0.6	-5.9	1.8	-6.5

Figure S2. Interaction energies for a 3.8 Å cluster around IB.



	N	Symop	R	Electron Density	E_ele	E_pol	E_dis	E_rep	E_tot
	1	-x, -y, -z	6.17	B3LYP/6-31G(d,p)	-14.4	-3.0	-65.4	59.7	-37.5
	1	-x, -y, -z	4.40	B3LYP/6-31G(d,p)	-14.8	-3.9	-83.9	68.6	-49.3
	2	x, -y, z+1/2	6.72	B3LYP/6-31G(d,p)	-13.9	-3.7	-18.3	21.4	-20.2
	2	-x+1/2, y+1/2, -z+1/2	12.12	B3LYP/6-31G(d,p)	-13.1	-2.0	-12.4	8.7	-20.7
	1	-x, y, -z+1/2	5.48	B3LYP/6-31G(d,p)	-97.4	-26.6	-50.7	126.1	-88.9
	2	x+1/2, y+1/2, z	15.11	B3LYP/6-31G(d,p)	-5.1	-1.3	-5.4	6.2	-7.2
	2	x+1/2, -y+1/2, z+1/2	15.25	B3LYP/6-31G(d,p)	-3.7	-0.8	-5.0	6.7	-4.8
	1	-x+1/2, -y+1/2, -z	12.01	B3LYP/6-31G(d,p)	2.4	-0.4	-1.7	0.1	0.7
	2	-x, y, -z+1/2	9.04	B3LYP/6-31G(d,p)	-3.0	-0.9	-8.0	3.4	-8.7
	2	x, -y, z+1/2	7.99	B3LYP/6-31G(d,p)	-1.9	-0.4	-9.4	4.4	-7.7

Figure S3. Interaction energies for a 3.8 Å cluster around II.