Development of anisotropic polarizable model for all-atom AMOEBA force fields

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Table S.1 Lattice parameters of refined experimental crystal structures optimized by three-type force fields. The units of lattice lengths *a, b* and *c*, packing similarity ($RMSD_{20}$) and crystal similarity (t-RMSD) are in Å and lattice angles of α β and γ in degree(°).

Models	Functionals	*a*	*b*	*c*	*A*	*β*	*γ*	$RMSD_{20}$
				NAPHTA06				
Exp.	-	5.940	7.832	8.108	90.00	114.32	90.00	-
NON-Polar	PBE	6.028	7.791	8.145	90.00	115.59	90.00	0.51
	M06	6.067	7.798	8.023	90.00	114.65	90.00	0.50
	M06-L	6.087	7.772	8.021	90.00	114.51	90.00	0.52
	CAM-B3LYP	6.043	7.798	8.077	90.00	115.08	90.00	0.52
	ωB97X-D	6.022	7.794	8.137	90.00	115.58	90.00	0.51

	B3LYP	6.044	7.800	8.080	90.00	115.10	90.00	0.52
	B2PLYP	6.023	7.803	8.115	90.00	115.43	90.00	0.49
ISO-Polar	PBE	5.979	7.802	8.179	90.00	115.73	90.00	0.49
	M06	6.026	7.809	8.032	90.00	114.60	90.00	0.43
	M06-L	6.058	7.782	8.019	90.00	114.42	90.00	0.49
	CAM-B3LYP	5.997	7.811	8.091	90.00	115.06	90.00	0.45
	ωB97X-D	5.973	7.801	8.159	90.00	115.59	90.00	0.48
	B3LYP	6.001	7.813	8.094	90.00	115.09	90.00	0.45
	B2PLYP	5.976	7.816	8.126	90.00	115.36	90.00	0.45
ANISO-Polar	PBE	5.960	7.827	8.181	90.00	115.82	90.00	0.47
	M06	6.003	7.838	8.037	90.00	114.75	90.00	0.41
	M06-L	6.041	7.806	8.021	90.00	114.53	90.00	0.44
	CAM-B3LYP	5.975	7.840	8.095	90.00	115.20	90.00	0.42
	ωB97X-D	5.950	7.832	8.167	90.00	115.75	90.00	0.46
	B3LYP	5.980	7.840	8.098	90.00	115.22	90.00	0.43
	B2PLYP	5.953	7.845	8.135	90.00	115.53	90.00	0.43
				ANTCEN01				
Exp.	-	6.002	8.443	9.256	90.00	102.27	90.00	-
NON-Polar	PBE	6.134	8.066	9.522	90.00	103.26	90.00	0.53
	M06	6.164	8.054	9.463	90.00	102.70	90.00	0.52
	M06-L	6.184	8.023	9.475	90.00	102.63	90.00	0.59
	CAM-B3LYP	6.140	8.064	9.495	90.00	103.01	90.00	0.53
	ωB97X-D	6.122	8.070	9.519	90.00	103.26	90.00	0.52
	B3LYP	6.144	8.065	9.494	90.00	103.00	90.00	0.51
	B2PLYP	6.120	8.075	9.516	90.00	103.23	90.00	0.49
ISO-Polar	PBE	6.082	8.105	9.528	90.00	103.34	90.00	0.47
	M06	6.118	8.093	9.453	90.00	102.67	90.00	0.47
	M06-L	6.149	8.054	9.462	90.00	102.59	90.00	0.51
	CAM-B3LYP	6.089	8.106	9.486	90.00	102.98	90.00	0.45
	ωB97X-D	6.069	8.111	9.513	90.00	103.21	90.00	0.44
	B3LYP	6.097	8.105	9.489	90.00	103.01	90.00	0.46
	B2PLYP	6.067	8.119	9.506	90.00	103.18	90.00	0.43
ANISO-Polar	PBE	6.047	8.124	9.572	90.00	103.72	90.00	0.44
	M06	6.078	8.128	9.482	90.00	103.00	90.00	0.42

M06-L	6.121	8.082	9.481	90.00	102.85	90.00	0.49
CAM-B3LYP	6.051	8.137	9.521	90.00	103.33	90.00	0.41
ωB97X-D	6.030	8.139	9.557	90.00	103.61	90.00	0.41
B3LYP	6.061	8.130	9.525	90.00	103.35	90.00	0.43
B2PLYP	6.028	8.147	9.549	90.00	103.56	90.00	0.40

Table S.2 The lattice parameters of all matched crystals from USPEX-predicted crystals using ANISO-Polar and ISO-Polar models. The units of lattice lengths , $RMSD_{20}$ and t-RMSD are in Å, lattice angles is in degree(°) and the Total energy of unit cell is in kcal/mol.

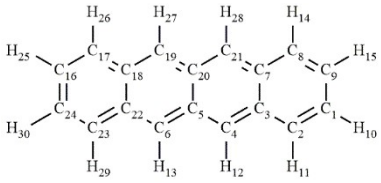
Models	No.	a	b	c	α	β	γ	$RMSD_{20}$	Energy
				NAPHTA06					
	Exp.	5.940	7.832	8.108	90.00	114.32	90.00	-	-
NON-Polar	Rank1	6.043	7.798	8.078	90.00	115.09	90.00	0.52	-21.86
ISO-Polar	Rank2	5.997	7.810	8.091	90.00	115.06	90.00	0.45	-22.89
ANISO-Polar	Rank4	5.974	7.841	8.096	90.07	115.21	90.08	0.42	-23.07
				ANTCEN01					
	Exp.	6.002	8.443	9.256	90.00	102.27	90.00	-	-
NON-Polar	Rank2	6.138	8.067	9.470	90.00	102.84	90.00	0.50	-28.90
ISO-Polar	Rank3	6.087	8.108	9.463	90.00	102.82	90.00	0.45	-30.29
ANISO-Polar	Rank2	6.049	8.140	9.500	90.14	103.18	90.11	0.40	-30.58
				TETCEN					
	Exp.	6.030	7.900	12.699	101.68	98.65	93.70	-	-
NON-Polar	Rank1	6.069	7.495	12.926	104.01	96.80	93.25	0.60	-33.63
ISO-Polar	Rank1	6.001	7.538	12.984	104.56	96.94	93.08	0.57	-35.74
ANISO-Polar	Rank1	5.967	7.586	12.990	104.70	97.09	92.94	0.53	-36.32
				PENCEN					
	Exp.	6.060	7.900	14.884	96.74	100.54	94.20	-	-
NON-Polar	Rank1	6.085	7.476	15.166	97.73	99.92	93.28	0.81	-44.06
ISO-Polar	Rank1	6.018	7.529	15.199	97.88	100.26	93.14	0.73	-46.49
ANISO-Polar	Rank1	6.002	7.760	14.721	96.49	98.75	93.77	0.28	-46.95

Table S.3. The distributed atomic polarizability tensors under the molecular standard coordinates. The unit of atomic polarizability α is in $4\pi\varepsilon_0 Å^3$.

Type	α_{xx}	α_{xy}	α_{xz}	α_{yz}	α_{yy}	α_{zz}	α_{iso}^{num}	α_{AMOEBA}
naphthalene								
1-C	1.711	-0.248	0.000	0.000	1.422	0.866	1.333	1.750
2-C	2.273	0.050	0.000	0.000	1.154	0.829	1.419	1.750
3-C	2.366	0.005	0.000	0.000	1.561	0.585	1.504	1.750
4-C	2.273	-0.050	0.000	0.000	1.154	0.829	1.419	1.750
5-C	1.711	0.248	0.000	0.000	1.422	0.866	1.332	1.750
6-H	0.722	0.290	0.000	0.000	0.288	0.142	0.384	0.696
7-H	0.147	0.073	0.000	0.000	0.741	0.140	0.343	0.696
8-H	0.147	-0.073	0.000	0.000	0.741	0.140	0.343	0.696
9-H	0.722	-0.290	0.000	0.000	0.288	0.142	0.384	0.696
10-C	1.711	-0.248	0.000	0.000	1.422	0.866	1.333	1.750
11-C	2.273	0.050	0.000	0.000	1.154	0.829	1.419	1.750
12-C	2.366	0.005	0.000	0.000	1.561	0.585	1.504	1.750
13-C	2.273	-0.050	0.000	0.000	1.154	0.829	1.419	1.750
14-C	1.711	0.248	0.000	0.000	1.422	0.866	1.332	1.750
15-H	0.722	0.290	0.000	0.000	0.288	0.142	0.384	0.696
16-H	0.147	0.073	0.000	0.000	0.741	0.140	0.343	0.696
17-H	0.147	-0.073	0.000	0.000	0.741	0.140	0.343	0.696
18-H	0.722	-0.290	0.000	0.000	0.288	0.142	0.384	0.696
$\sum\alpha$	24.144	0.010	0.000	0.000	17.542	9.078	16.922	-
anthracene								
1-C	1.992	-0.289	0.000	0.000	1.352	0.861	1.402	1.750
2-C	2.704	0.087	0.000	0.000	1.147	0.823	1.558	1.750
3-C	3.031	-0.065	0.000	0.000	1.536	0.579	1.715	1.750

4-C	3.177	-0.001	0.000	0.000	1.098	0.771	1.682	1.750
5-C	3.031	0.065	0.000	0.000	1.536	0.579	1.715	1.750
6-C	2.704	-0.087	0.000	0.000	1.147	0.823	1.558	1.750
7-C	1.992	0.289	0.000	0.000	1.352	0.861	1.402	1.750
8-H	0.805	0.306	0.000	0.000	0.280	0.142	0.409	0.696
9-H	0.156	0.116	0.000	0.000	0.729	0.140	0.342	0.696
10-H	0.133	0.000	0.000	0.000	0.716	0.138	0.329	0.696
11-H	0.156	-0.116	0.000	0.000	0.729	0.140	0.342	0.696
12-H	0.805	-0.306	0.000	0.000	0.280	0.142	0.409	0.696
13-C	1.992	-0.289	0.000	0.000	1.352	0.861	1.402	1.750
14-C	2.704	0.087	0.000	0.000	1.147	0.823	1.558	1.750
15-C	3.031	-0.065	0.000	0.000	1.536	0.579	1.715	1.750
16-C	3.177	-0.001	0.000	0.000	1.098	0.771	1.682	1.750
17-C	3.031	0.065	0.000	0.000	1.536	0.579	1.715	1.750
18-C	2.704	-0.087	0.000	0.000	1.147	0.823	1.558	1.750
19-C	1.992	0.289	0.000	0.000	1.352	0.861	1.402	1.750
20-H	0.805	0.306	0.000	0.000	0.280	0.142	0.409	0.409
21-H	0.156	0.116	0.000	0.000	0.729	0.140	0.342	0.696
22-H	0.133	0.000	0.000	0.000	0.716	0.138	0.329	0.696
23-H	0.156	-0.116	0.000	0.000	0.729	0.140	0.342	0.696
24-H	0.805	-0.306	0.000	0.000	0.280	0.142	0.409	0.696
$\sum\alpha$	41.372	-0.002	0.000	0.000	23.804	11.998	25.726	-

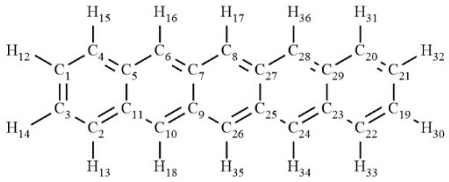
tetracene



1-C	2.175	-0.308	0.000	0.000	1.295	0.854	1.441	1.750
2-C	2.979	0.113	0.000	0.000	1.135	0.815	1.643	1.750
3-C	3.469	-0.101	0.000	0.000	1.507	0.573	1.850	1.750
4-C	3.752	0.028	0.000	0.000	1.095	0.760	1.869	1.750
5-C	3.815	0.004	0.000	0.000	1.560	0.565	1.980	1.750
6-C	3.752	-0.028	0.000	0.000	1.095	0.760	1.869	1.750
7-C	3.469	0.101	0.000	0.000	1.507	0.573	1.850	1.750
8-C	2.979	-0.113	0.000	0.000	1.135	0.815	1.643	1.750

9-C	2.175	0.308	0.000	0.000	1.295	0.854	1.441	1.750
10-H	0.870	0.318	0.000	0.000	0.275	0.143	0.429	0.696
11-H	0.165	0.144	0.000	0.000	0.721	0.140	0.342	0.696
12-H	0.139	0.040	0.000	0.000	0.707	0.138	0.328	0.696
13-H	0.139	-0.040	0.000	0.000	0.707	0.138	0.328	0.696
14-H	0.165	-0.144	0.000	0.000	0.721	0.140	0.342	0.696
15-H	0.870	-0.318	0.000	0.000	0.275	0.143	0.429	0.696
16-C	2.175	-0.308	0.000	0.000	1.295	0.854	1.441	1.750
17-C	2.979	0.113	0.000	0.000	1.135	0.815	1.643	1.750
18-C	3.469	-0.101	0.000	0.000	1.507	0.573	1.850	1.750
19-C	3.752	0.028	0.000	0.000	1.095	0.760	1.869	1.750
20-C	3.815	0.004	0.000	0.000	1.560	0.565	1.980	1.750
21-C	3.752	-0.028	0.000	0.000	1.095	0.760	1.869	1.750
22-C	3.469	0.101	0.000	0.000	1.507	0.573	1.850	1.750
23-C	2.979	-0.113	0.000	0.000	1.135	0.815	1.643	1.750
24-C	2.175	0.308	0.000	0.000	1.295	0.854	1.441	1.750
25-H	0.870	0.318	0.000	0.000	0.275	0.143	0.429	0.696
26-H	0.165	0.144	0.000	0.000	0.721	0.140	0.342	0.696
27-H	0.139	0.040	0.000	0.000	0.707	0.138	0.328	0.696
28-H	0.139	-0.040	0.000	0.000	0.707	0.138	0.328	0.696
29-H	0.165	-0.144	0.000	0.000	0.721	0.140	0.342	0.696
30-H	0.870	-0.318	0.000	0.000	0.275	0.143	0.429	0.696
$\sum\alpha$	61.826	0.008	0.000	0.000	30.06	14.822	35.568	-

pentacene



1-C	2.337	-0.330	0.000	0.000	1.263	0.853	1.484	1.750
2-C	3.225	-0.133	0.000	0.000	1.133	0.812	1.723	1.750
3-C	2.337	0.330	0.000	0.000	1.263	0.853	1.484	1.750
4-C	3.225	0.133	0.000	0.000	1.133	0.812	1.723	1.750
5-C	3.841	-0.131	0.000	0.000	1.505	0.573	1.973	1.750
6-C	4.219	0.045	0.000	0.000	1.103	0.756	2.026	1.750
7-C	4.448	-0.045	0.000	0.000	1.602	0.564	2.205	1.750

8-C	4.529	0.002	0.000	0.000	1.117	0.753	2.133	1.750
9-C	4.448	0.045	0.000	0.000	1.602	0.564	2.205	1.750
10-C	4.219	-0.045	0.000	0.000	1.103	0.756	2.026	1.750
11-C	3.841	0.131	0.000	0.000	1.505	0.573	1.973	1.750
12-H	0.923	0.329	0.000	0.000	0.272	0.143	0.446	0.696
13-H	0.173	-0.167	0.000	0.000	0.716	0.140	0.343	0.696
14-H	0.923	-0.329	0.000	0.000	0.272	0.143	0.446	0.696
15-H	0.173	0.167	0.000	0.000	0.716	0.140	0.343	0.696
16-H	0.145	0.069	0.000	0.000	0.703	0.137	0.328	0.696
17-H	0.142	0.000	0.000	0.000	0.703	0.137	0.327	0.696
18-H	0.145	-0.069	0.000	0.000	0.703	0.137	0.328	0.696
19-C	2.337	-0.330	0.000	0.000	1.263	0.853	1.484	1.750
20-C	3.225	-0.133	0.000	0.000	1.133	0.812	1.723	1.750
21-C	2.337	0.330	0.000	0.000	1.263	0.853	1.484	1.750
22-C	3.225	0.133	0.000	0.000	1.133	0.812	1.723	1.750
23-C	3.841	-0.131	0.000	0.000	1.505	0.573	1.973	1.750
24-C	4.219	0.045	0.000	0.000	1.103	0.756	2.026	1.750
25-C	4.448	-0.045	0.000	0.000	1.602	0.564	2.205	1.750
26-C	4.529	0.002	0.000	0.000	1.117	0.753	2.133	1.750
27-C	4.448	0.045	0.000	0.000	1.602	0.564	2.205	1.750
28-C	4.219	-0.045	0.000	0.000	1.103	0.756	2.026	1.750
29-C	3.841	0.131	0.000	0.000	1.505	0.573	1.973	1.750
30-H	0.923	0.329	0.000	0.000	0.272	0.143	0.446	0.696
31-H	0.173	-0.167	0.000	0.000	0.716	0.140	0.343	0.696
32-H	0.923	-0.329	0.000	0.000	0.272	0.143	0.446	0.696
33-H	0.173	0.167	0.000	0.000	0.716	0.140	0.343	0.696
34-H	0.145	0.069	0.000	0.000	0.703	0.137	0.328	0.696
35-H	0.142	0.000	0.000	0.000	0.703	0.137	0.327	0.696
36-H	0.145	-0.069	0.000	0.000	0.703	0.137	0.328	0.696
$\sum\alpha$	86.586	0.004	0.000	0.000	36.828	17.692	47.032	-

Table S.4. Energy decomposition analysis on the basis of the optimized experimental crystals using NON-Polar, ISO-Polar and ANISO-Polar models. The unit of energy is in kcal mol^{-1}.

Energy terms	NON-Polar	ISO-Polar	ANISO-Polar
naphthalene			

Total Potential	-21.8597	-22.8852	-23.0695
Bond stretching	0.1432	0.1399	0.1380
Angle bending	0.0236	0.0270	0.0289
Stretch-bend	0.0008	0.0010	0.0010
Out-of-plane bend	0.0003	0.0003	0.0003
Torsional angle	0.0055	0.0069	0.0070
vdW interaction	-20.8278	-20.7629	-20.7192
Electrostatic interaction	-1.2053	-1.2453	-1.2691
Polarization	-	-1.0520	-1.2564
	anthracene		
Total Potential	-27.6049	-28.9887	-29.2703
Bond stretching	0.2389	0.2357	0.2338
Angle bending	0.0292	0.0338	0.0375
Stretch-bend	0.0010	0.0012	0.0012
Out-of-plane bend	0.0012	0.0012	0.0014
Torsional angle	0.0156	0.0180	0.0177
vdW interaction	-27.3519	-27.2061	-27.0755
Electrostatic interaction	-0.5389	-0.6489	-0.7272
Polarization	-	-1.4235	-1.7592
	tetracene		
Total Potential	-33.6150	-35.7333	-36.3028
Bond stretching	0.3616	0.3561	0.3504
Angle bending	0.0504	0.0532	0.0516
Stretch-bend	0.0029	0.0031	0.0029
Out-of-plane bend	0.0011	0.0012	0.0011
Torsional angle	0.0098	0.0094	0.0092
vdW interaction	-34.1462	-33.8003	-33.5814
Electrostatic interaction	-0.1054	-0.1622	-0.3038
Polarization	-	-2.1938	-2.8329
	pentacene		
Total Potential	-44.3779	-46.8123	-47.2640
Bond stretching	0.4191	0.4136	0.4056
Angle bending	0.0568	0.0594	0.0539
Stretch-bend	0.0030	0.0033	0.0024
Out-of-plane bend	0.0019	0.0021	0.0012
Torsional angle	0.0148	0.0142	0.0100
vdW interaction	-41.7130	-41.3075	-41.0615
Electrostatic interaction	-3.1605	-3.4774	-3.5743
Polarization	-	-2.5198	-3.1013

Table S.5 Molecular polarizability of naphthalene and anthracene calculated from different density functionals coupled with 6-311+G(d,p) basis set. (The unit of polarizability α is in $4\pi\varepsilon_0 Å^3$)

	naphthalene					anthracene				
	α_{xx}	α_{yy}	α_{zz}	α_{iso}	k	α_{xx}	α_{yy}	α_{zz}	α_{iso}	k
PBE	25.16	18.13	9.17	17.49	0.265	43.96	24.56	11.98	26.83	0.347
M06	24.80	17.86	9.22	17.29	0.261	42.85	24.27	12.21	26.44	0.337
M06-L	24.42	17.53	8.78	16.91	0.268	42.61	23.79	11.65	26.02	0.346
CAM-B3LYP	24.14	17.54	9.08	16.92	0.258	41.37	23.80	12.00	25.72	0.332
ωB97X-D	24.08	17.54	9.06	16.90	0.258	41.17	23.80	12.02	25.66	0.330
B3LYP	24.74	17.84	9.15	17.24	0.262	42.85	24.17	12.09	26.37	0.339
B2PLYP	24.44	17.7	9.16	17.10	0.259	42.15	23.92	12.12	26.06	0.335