Supplementary Information

Investigation of the electronic and optical properties of Al_{13}-dianhydride complexes by (time-dependent) density functional theory

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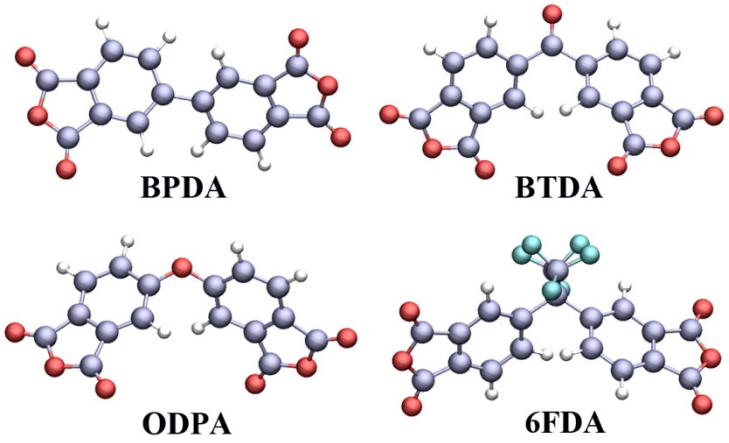

Fig. S1 Structures of the BPDA, BTDA, ODPA, and 6FDA calculated at the PBE1PBE-D3/def2-SVP level of theory.

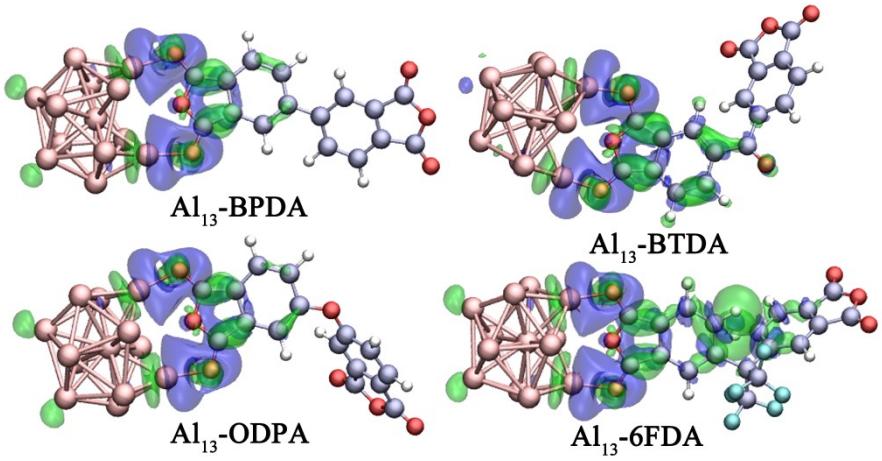

Fig. S2 Charge density difference maps of Al_{13}-X, with the isosurface value of 0.002 a.u.

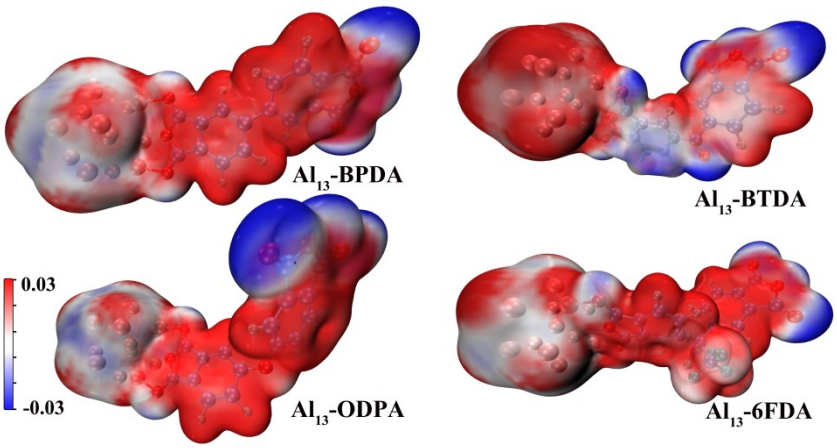

Fig. S3 Electrostatic potential maps (ESP) for the Al_{13}-X (X = BPDA, BTDA, ODPA, and 6FDA), where the blue region denotes the negative, while the red region represents the positive counterpart.

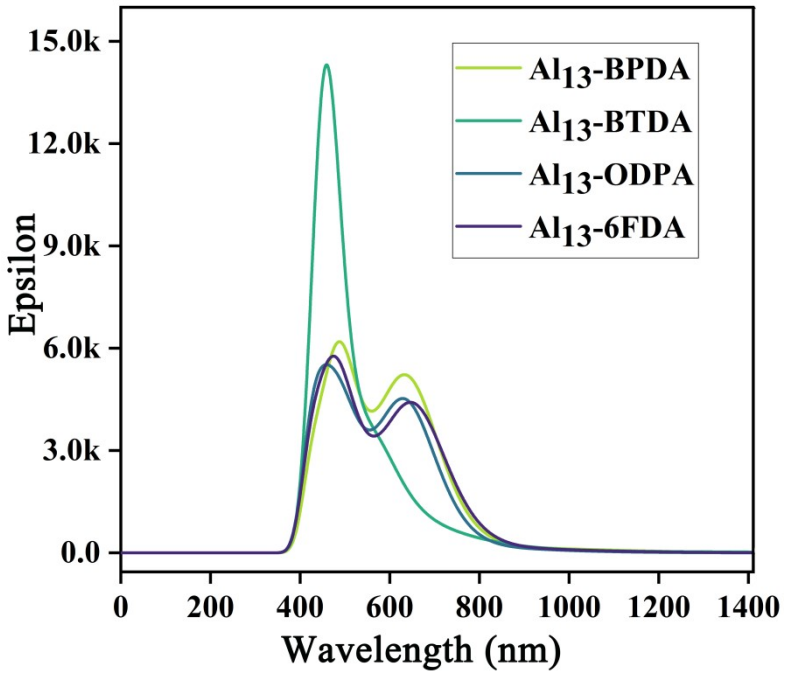

Fig. S4 Simulated UV-vis absorption spectrum of the Al_{13}-X (X = BPDA, BTDA, ODPA, and 6FDA) calculated at the TD-CAM-B3LYP/6-31+G(d) level.

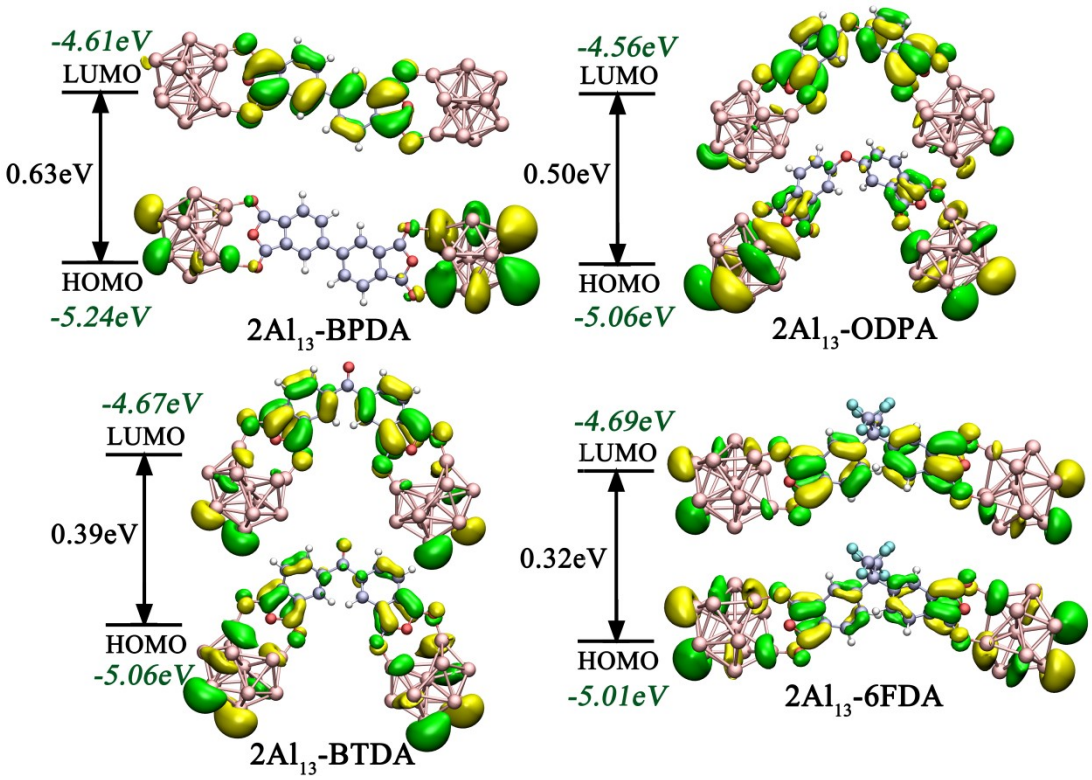

Fig. S5 HOMOs and LUMOs of the studied molecules. Frontier molecular orbital energies (in eV) and HOMO-LUMO gap (in eV) are given.

Table S1 The components of polarizability (in a.u.), isotropic average polarizability (α_{iso}, in a.u.), anisotropic polarizability (α_{aniso}, in a.u.), components of the first hyperpolarizability (in a.u.), and total first hyperpolatizability (β_{tot}, in a.u.)

	Al_{13}-BPDA	Al_{13}-BTDA	Al_{13}-ODPA	Al_{13}-6FDA
α_{xx}	1042	885	899	1029
α_{yy}	673	700	722	667
α_{zz}	618	631	649	690
α_{iso}	778	739	757	795
α_{aniso}	399	227	221	351
β_{xxx}	-10995	-3591	-3550	-7333
β_{yyy}	142	360	-9	102
β_{zzz}	148	97	-194	55
β_{X}	-9133	-2780	-2264	-5617
β_{Y}	150	2496	243	280
β_{Z}	-338	-545	293	-504
β_{tot}	9141	3775	2297	5646

Table S2 Frontier molecular orbital energies (E_H and E_L, in eV), HOMO-LUMO gap (E_{gap}, in eV), isotropic average polarizability (α_{iso}, in a.u.), and total first hyperpolatizability (β_{tot}, in a.u.), excitation energy (ΔE, in eV), and oscillator strength (f_{os}) of BPDA, BTDA, ODPA, 6FDA, and Al_{13}

	BPDA	BTDA	ODPA	6FDA	$A1_{13}$
E_H	-8.23	-8.49	-7.92	-8.79	-5.94
E_L	-3.11	-3.60	-3.02	-3.21	-3.03
E_{gap}	4.92	4.89	4.90	5.58	2.91[a]
α_{iso}	203	210	202	230	518
β_{tot}	11	88	427	346	0
ΔE	5.72	4.90	4.49	6.02	2.15
f_{os}	0.977	0.232	0.210	1.598	0.011

[a]HOMO-LUMO gap of alpha orbital

Table S3 The components of polarizability (in a.u.), isotropic average polarizability (α_{iso}, in a.u.), components of the first hyperpolarizability (in a.u.), and total first hyperpolatizability (β_{tot}, in a.u.) of $2Al_{13}$-X (X = BPDA, BTDA, ODPA, and 6FDA)

	$2Al_{13}$-BPDA	$2Al_{13}$-BTDA	$2Al_{13}$-ODPA	$2Al_{13}$-6FDA
α_{xx}	4409	5866	5518	10421
α_{yy}	1144	2078	1695	1266
α_{zz}	1104	1063	1110	1143
α_{iso}	2220	3003	2775	4277
β_{xxx}	125464	-21	-351420	22468
β_{xxy}	-963	-83024	-488612	-53303
β_{xyy}	-107	-2	-9596	-5903
β_{yyy}	89	3072	-72113	4683
β_{xxz}	39703	-5	28590	25359
β_{xyz}	583	6912	24714	1608
β_{yyz}	-323	2	3049	-146
β_{xzz}	662	2	-1583	-527
β_{yzz}	-79	3532	1557	1291
β_{zzz}	-345	0.6	57	-1695
β_{tot}	131930	76420	667196	55230

Cartesian Coordinates

1. **Al_{13}-BPDA**

C 1.53746300 1.48349100 -0.38547400

C 1.78517200 0.10670600 -0.05799200

C 3.09091700 -0.40054500 -0.01742000

C 4.15070300 0.45590700 -0.29778500

C 3.89025400 1.82391600 -0.61905000

C 2.61338400 2.34257400 -0.66904200

C 0.13566100 1.66789800 -0.35197000

C 0.52132600 -0.49471700 0.16562100

H 3.26266500 -1.44274700 0.25814200

H 4.73367900 2.47391200 -0.86078900

H 2.43802200 3.38772400 -0.93001500

O -0.41684100 0.47170800 -0.00838700

O 0.05964600 -1.63548900 0.43824200

O -0.69719200 2.59234700 -0.55894000

C 8.14786600 -1.01401300 -0.19739500

C 7.85918900 0.26567700 0.25523400

C 6.57441300 0.78133400 0.23646000

C 5.54463300 -0.03762300 -0.25967600

C 5.85414100 -1.33587200 -0.72060400

C 7.15182900 -1.84287900 -0.69558800

C 9.60527300 -1.22884500 -0.03054200

C 9.13266100 0.87261800 0.71865400

H 6.37639000 1.78350600 0.62216900

H 5.05270000 -1.95225700 -1.13422400

H 7.38122900 -2.84569300 -1.06129000

O 10.12198800 -0.06812700 0.51813300

O 9.34736500 1.94689100 1.17999200

O 10.28023000 -2.17267800 -0.28672100

Al -5.77112400 0.39812200 2.11290500

Al -3.12212400 1.11617400 2.17945700

Al -4.97319700 2.41690800 0.46534700

Al -6.65237500 0.74465500 -0.64921900

Al -6.16935400 -1.84760600 0.88519000

Al -3.69840600 -1.58285500 2.28764800

Al -2.53123700 2.03369400 -0.39244300

Al -4.31155200 1.31205800 -2.18175500

Al -5.58763200 -1.24463800 -1.92184000

Al -4.08784200 -2.86718000 -0.33290300

Al -1.87072100 -1.69212500 0.41024000

Al -2.85420200 -1.03285600 -2.11864600

Al -4.09142900 -0.15092200 0.05654700

2. **Al_{13}-BTDA**

C -8.14103300 -2.49001800 0.29428000

C -7.50287000 -1.15971600 0.44497300

C -6.43657100 -1.10620500 -0.44221400

C -6.39362500 -2.39878300 -1.16744300

C -7.02107100 1.05055800 1.16001700

C -5.91807300 1.10255500 0.28647400

C -7.82208100 -0.08437400 1.26467800

C -5.62188900 0.01227800 -0.54395700

O -9.07716500 -2.96455900 0.85313800

O -5.65177200 -2.78588600 -2.01237500

O -7.43100500 -3.17033900 -0.67755200

H -8.66950000 -0.13073100 1.95152900

H -4.79873600 0.04282600 -1.26020300

C 0.43429200 2.43779500 -0.48953800

C -0.91535400 2.65976200 -0.40525000

C -1.51128800 1.41530600 0.09986400

C -0.47148400 0.53001400 0.29157900

C -3.10824300 3.64333800 -0.48248600

C -3.70249900 2.40356600 -0.02266300

C -1.76881100 3.77409600 -0.68204400

C -2.91361600 1.31478200 0.27617400

O 1.52853800 3.06980800 -0.85819100

O -0.28754800 -0.70675600 0.68893600

O 0.67496600 1.15978000 -0.06252700

H -1.34130500 4.71251100 -1.04095800

H -3.33837600 0.38993100 0.67109900

C -5.16420800 2.40559600 0.20986100

O -5.78616800 3.44335200 0.34185300

H -3.78826200 4.47740900 -0.66335300

H -7.23625800 1.94167300 1.75388700

Al 3.08821800 2.21540900 -0.79806700

Al 4.50377400 0.70874800 -2.36409400

Al 2.40651200 -1.05650500 -2.10471800

Al 1.40597300 -1.28784900 0.59669200

Al 3.01171800 0.67174600 2.37012300

Al 4.99578300 1.92183800 0.93998400

Al 5.05647700 -1.87849600 -1.90480100

Al 3.12080300 -3.03908600 -0.34880200

Al 3.38387200 -2.01108500 2.21560700

Al 5.61531800 -0.36890200 2.16111300

Al 6.41973400 0.06034400 -0.48938800

Al 5.58336000 -2.41931100 0.59519200

Al 3.81493600 -0.35224300 0.04253500

3. **Al_{13}-ODPA**

C -8.49492900 -2.12335600 -0.28046900

C -7.73263100 -0.87443300 -0.50769500

C -6.76733900 -0.78632500 0.48633100

C -6.91348900 -1.98226500 1.35638800

C -6.97486900 1.18396700 -1.42166200

C -6.00072300 1.26166700 -0.41356700

C -7.86015500 0.11059600 -1.47946200

C -5.88057100 0.27384800 0.57159100

O -9.40423000 -2.59419500 -0.88315800

O -6.29766800 -2.30621100 2.32000400

O -7.95226000 -2.72742700 0.84237900

H -8.62153300 0.04076200 -2.25881700

H -5.13546000 0.33464100 1.36693100

C 0.21100400 2.33896100 0.54419200

C -1.17992800 2.55280100 0.40296000

C -1.72669400 1.36474100 -0.19258800

C -0.64543500 0.47299300 -0.39082800

C -3.36300700 3.52254500 0.44224700

C -3.89620800 2.34143400 -0.14301100

C -2.01812600 3.63850100 0.71533300

C -3.09816800 1.25869100 -0.47528300

O 1.21967200 2.96609200 0.96792100

O -0.45631700 -0.68849200 -0.84932500

O 0.47619900 1.09693300 0.06261900

H -1.61082700 4.54496800 1.16658900

H -3.50868600 0.36225700 -0.94179600

O -5.22994000 2.38393100 -0.40409000

H -4.05934600 4.33213400 0.66643700

H -7.01532700 1.99297400 -2.15330300

Al 4.90875900 -2.18706400 1.72102800

Al 2.30124800 -1.33317200 1.87966300

Al 3.17846700 -3.06807400 -0.18806900

Al 5.53459600 -2.40618800 -1.12323700

Al 6.51750000 -0.33655800 0.88402700

Al 4.27446500 0.51779900 2.42923700

Al 1.37748800 -1.25868700 -0.75851200

Al 3.31589800 -1.28305700 -2.52582100

Al 5.78429100 0.04733300 -1.91880700

Al 5.37917600 1.87436200 0.06025900

Al 2.86345300 1.97844300 0.77124100

Al 3.39706900 1.41049700 -1.91632400

Al 3.87183400 -0.41555400 -0.05189400

4. **Al_{13}-6FDA**

C -8.34784900 2.90554800 0.82760900

C -7.17888000 1.99526300 0.72737300

C -7.55386100 0.91926700 -0.06085600

C -8.96530600 1.13398300 -0.46866000

C -5.02193200 1.04177400 0.97493800

C -5.39131600 -0.05290600 0.16809500

C -5.90482000 2.07913600 1.26881500

C -6.68999300 -0.12569400 -0.35120600

O -8.46945500 3.93951200 1.39978800

O -9.68006600 0.46626600 -1.14275600

O -9.36761600 2.32948500 0.09523500

H -5.60739400 2.92118900 1.89651500

H -7.03824300 -0.95787900 -0.96133200

C 0.85461000 0.93347800 -1.15510900

C -0.51220100 0.58689100 -1.02887700

C -0.58079300 -0.50895900 -0.10566000

C 0.74814600 -0.79154500 0.29682400

C -2.88763600 0.50598300 -1.24550500

C -2.96624300 -0.57638600 -0.31711200

C -1.69064200 1.08805800 -1.60610200

C -1.80839600 -1.09443400 0.23991800

O 1.55950400 1.77051200 -1.78089400

O 1.34405700 -1.59289400 1.06431300

O 1.55576900 0.08719800 -0.35175900

H -1.65861400 1.91390000 -2.31862000

H -1.81735500 -1.93621500 0.93021000

C -4.39337900 -2.02861400 1.25237800

F -5.64058200 -2.34934100 1.56816500

F -3.70464700 -3.16276400 1.12506100

F -3.87529400 -1.35296600 2.27811600

C -4.68994000 -2.07741900 -1.25204200

F -3.67979500 -2.89123700 -1.52613000

F -5.76776700 -2.83047900 -1.03648400

F -4.92193300 -1.33638600 -2.33583600

C -4.35369700 -1.16460500 -0.03898100

H -4.01022600 1.07743300 1.38326400

H -3.81051300 0.88538000 -1.68663900

Al 3.25319600 -1.31317600 1.13128300

Al 5.27399900 -2.46696000 -0.07472900

Al 5.46522900 -1.05383300 2.50568400

Al 3.85331800 1.24292900 2.08508500

Al 3.44643200 1.59971800 -1.42155700

Al 4.42373500 -0.89990300 -2.18549100

Al 7.56754100 -1.10809600 0.94857600

Al 6.59505500 1.39382200 2.11599400

Al 5.05245100 2.88133200 0.20815200

Al 5.92898700 1.50793300 -2.24410100

Al 7.10365400 -0.85980000 -1.58687500

Al 7.61037500 1.69497600 -0.24704600

Al 5.25062400 0.21115000 0.07842100