Electronic Supplementary Information (ESI)

Interaction energies and stabilities of heteroatom-containing aromatic compounds on graphite

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1. Estimated CCSD(T) level intermolecular interaction energies at the basis set limit

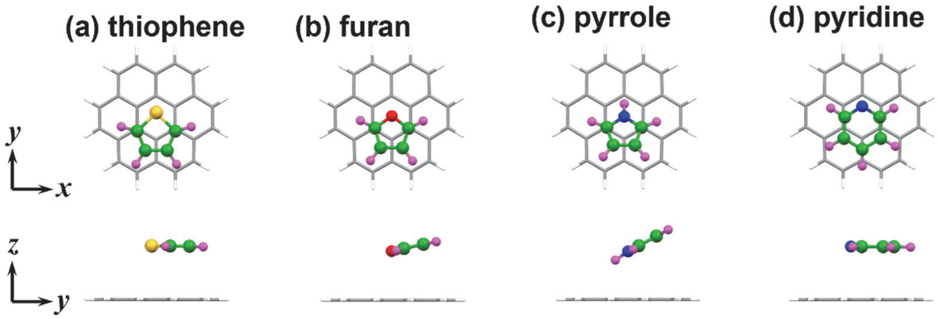


Fig. S1 Optimised geometries of coronene complexes with (a) thiophene, (b) furan, (c) pyrrole and (d) pyridine, viewed from different directions. The carbon, hydrogen, sulphur, oxygen and nitrogen atoms of adsorbed molecules are coloured in green, pink, yellow, red and blue, respectively.

Table S1 Calculated interaction energies for coronene complexes with thiophene, furan, pyrrole and pyridine.[a]

Adsorbate	$E_{\text{B3LYP-D3}}$ [b]	$E_{\text{CCSD(T)(limit)}}$ [c]	Difference [d]	Relative error [e]
thiophene	-7.17	-6.90	0.27	3.9
furan	-5.73	-5.88	0.15	2.6
pyrrole	-7.07	-6.48	0.59	9.2
pyridine	-7.22	-7.17	0.05	0.7

[a] Energy in kcal mol^{-1}.

[b] B3LYP-D3/6-311G** level interaction energy.

[c] Estimated CCSD(T) level interaction energy at the basis set limit. The calculations were performed based on the method as reported previously.[S1]

[d] $|E_{\text{B3LYP-D3}} - E_{\text{ccsd(T)limit.}}|$

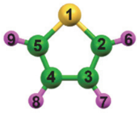
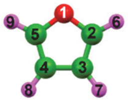
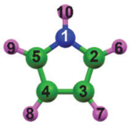
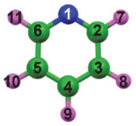
[e] Relative error in %.

S1 (a) S. Tsuzuki and T. Uchimaru, *Phys. Chem. Chem. Phys.*, 2020, **22**, 22508.; (b) Y. Kikkawa and S. Tsuzuki, *Phys. Chem. Chem. Phys.*, 2023, **25**, 11331.

2. Small molecular geometry changes upon adsorption onto $C_{96}H_{24}$

The changes in bond lengths, bond angles, and dihedral angles during the geometry optimizations of the $C_{96}H_{24}$ complexes with HACs (thiophene, furan, pyrrole, and pyridine) were analysed. Minimal variations were observed in the bond lengths and bond angles, limited to changes in the fourth and first decimal places, respectively (data not shown). As shown in Table S2, the variations in the dihedral angles of the aromatic rings were below 0.5°, and the torsional angles involving hydrogen atoms varied by less than 1.8°, except for the pyrrole C–C–N–H dihedral angle (6.7°). These results indicate that the geometric changes of HACs upon adsorption onto $C_{96}H_{24}$ are negligible.

Table S2 Dihedral angle changes of HACs upon adsorption onto $C_{96}H_{24}$

	Dihedral angle	Variation / °
thiophene	C3–C4–C5–S1	0.02
	C3–C4–C5–H9	1.41
	C4–C3–C2–H6	
	C2–C3–C4–H8	1.46
	C5–C4–C3–H7	
furan	C3–C4–C5–O1	0.08
	C3–C4–C5–H9	1.52
	C4–C3–C2–H6	
	C2–C3–C4–H8	1.28
	C5–C4–C3–H7	
pyrrole	C3–C4–C5–N1	0.45
	C3–C4–C5–H9	1.79
	C4–C3–C2–H6	1.84
	C3–C2–N1–H10	6.71
pyridine	C4–C3–C2–N1	0.14
	C4–C3–C2–H7	1.09
	C4–C5–C6–H11	
	C5–C4–C3–H8	1.30
	C3–C4–C5–H10	
	C2–C3–C4–H9	1.48

3. Intermolecular interaction energies of $C_{96}H_{24}$-HACs and $C_{96}H_{24}$-benzene complexes based on symmetry-adapted perturbation theory (SAPT) calculations

The SAPT calculations for $C_{96}H_{24}$-HACs and $C_{96}H_{24}$-benzene complexes were performed to reveal the contributions of the electrostatic (E_{es}), induction (E_{ind}), exchange-repulsion (E_{ex}) and dispersion (E_{disp}) interactions. The calculated E_{es}, E_{ind}, E_{ex}, E_{disp} and E_{int} using the 6-31G* basis set are listed in Table S3. The E_{es} calculated for the $C_{96}H_{24}$-HACs complexes (-4.0 to -5.0 kcal/mol) are close to that for the $C_{96}H_{24}$-benzene complex (-4.9 kcal/mol). The E_{ind} calculated for the $C_{96}H_{24}$-HACs complexes (-0.7 to -1.2 kcal/mol) are small. They are close to the E_{ind} calculated for the $C_{96}H_{24}$-benzene complex (-0.8 kcal/mol, respectively). The E_{disp} calculated for the $C_{96}H_{24}$-HACs complexes are larger (more negative) than the E_{es} and E_{ind} as well as the $C_{96}H_{24}$-benzene complex, indicating that the dispersion interactions are the primary source of the attraction in the $C_{96}H_{24}$-HACs and $C_{96}H_{24}$-benzene complexes. These results indicate that the effects of heteroatoms of HACs on the electrostatic and induction interactions between HACs and $C_{96}H_{24}$ are small, suggesting that the nature of the interactions of HACs with graphene is similar to that of benzene.

Table S3 Contribution of each energy term and total intermolecular interaction energies for $C_{96}H_{24}$-HACs and $C_{96}H_{24}$-benzene complexes obtained by SAPT calculations.[a]

Adsorbate	E_{es}[b]	E_{ex}[c]	E_{ind}[d]	E_{disp}[e]	E_{int}[f]
thiophene	-4.98	12.19	-0.84	-8.87	-2.51
furan	-4.00	9.88	-0.71	-7.45	-2.29
pyrrole	-4.82	11.34	-1.15	-7.98	-2.61
pyridine	-4.63	11.86	-0.92	-9.34	-3.03
benzene	-4.86	12.33	-0.83	-9.49	-2.86

[a] Energy in kcal mol^{-1}. The 6-31G* basis set was used [b] Electrostatic. [c] Exchange-repulsion.
[d] Induction. [e] Dispersion. [f] Total interaction energy.

4. Optimised geometries and intermolecular interaction energies of edge-on oriented thiophene, furan, pyrrole, and pyridine on $C_{96}H_{24}$

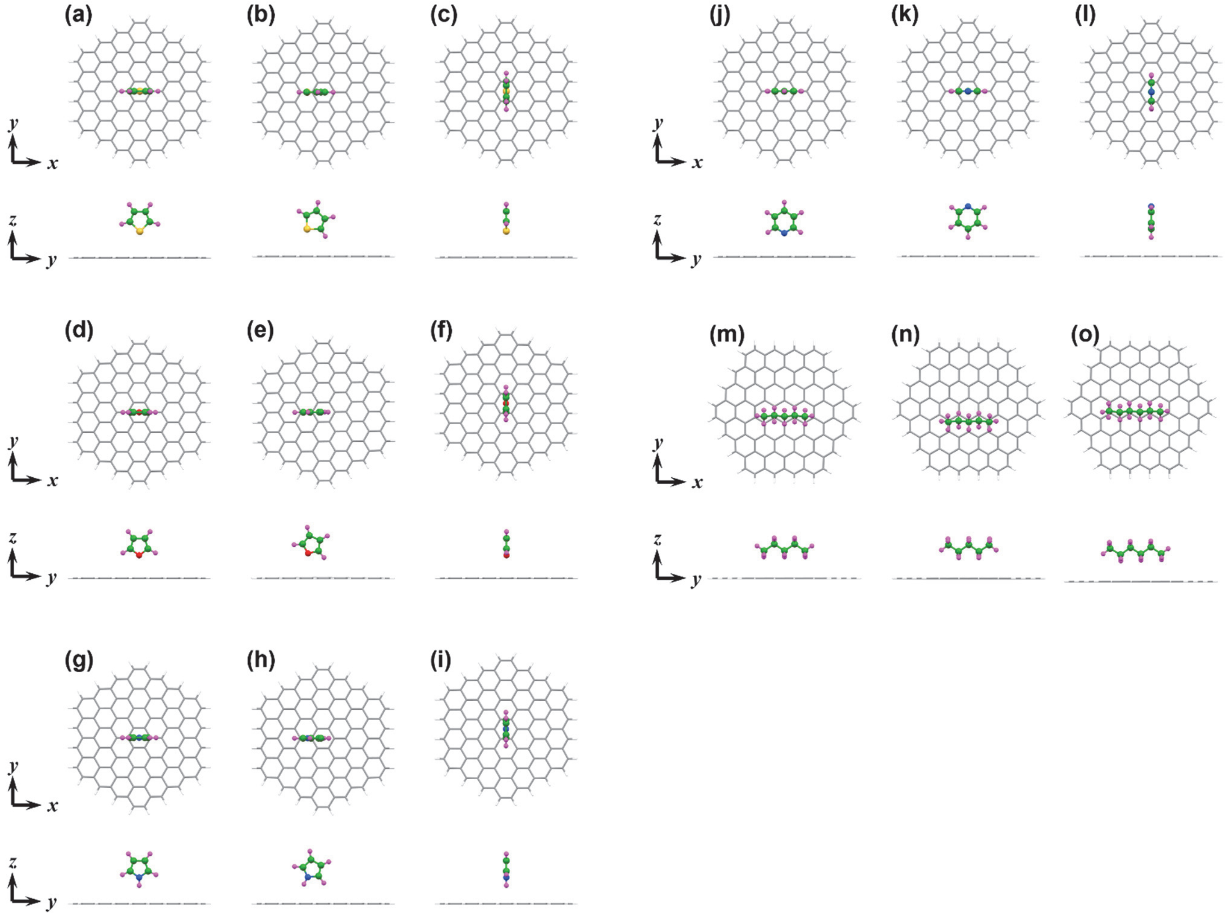


Fig. S2 Optimised geometries of $C_{96}H_{24}$ complexes with edge-on oriented (a-c) thiophene, (d-f) furan, (g-i) pyrrole, (j-l) pyridine, (m,n) *n*-pentane and (o) *n*-hexane, viewed from different directions. The carbon, hydrogen, sulphur, oxygen and nitrogen atoms of adsorbed molecules are coloured in green, pink, yellow, red and blue, respectively.

Table S4 Calculated interaction energies for $C_{96}H_{24}$ complexes with edge-on oriented (a-c) thiophene, (d-f) furan, (g-i) pyrrole, (j-l) pyridine, (m,n) *n*-pentane, and (o) *n*-hexane.

Adsorbate	Geometry [a]	E_{int} [b]
thiophene	a	-5.20
	b	-6.50
	c	-5.20
Furan	d	-5.38
	e	-4.90
	f	-5.34
pyrrole	g	-6.17
	h	-6.74
	i	-6.16
pyridine	j	-6.11
	k	-5.65
	l	-5.64
n-pentane	m	-9.76
	n	-8.70
n-hexane	o	-10.93

[a] Geometries of complexes are shown in Fig. S2.

[b] Energy in kcal mol^{-1}.

5. Optimised geometries and intermolecular interaction energies of $C_{96}H_{24}$ complexes with HACs with a higher number of fused benzenes

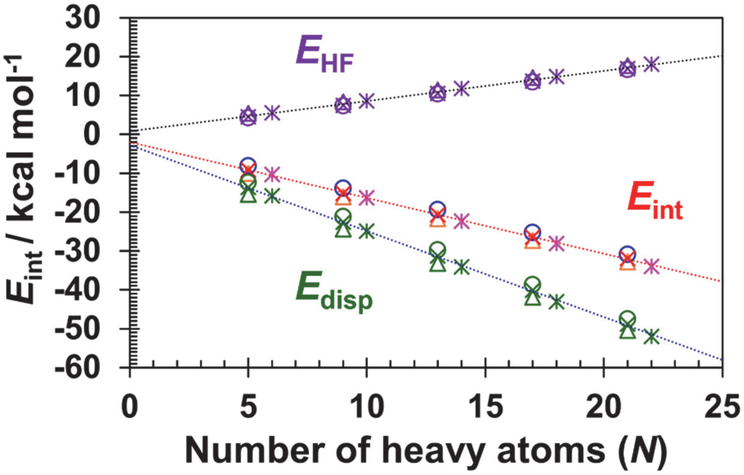


Fig. S3 Plots of E_{int}, E_{HF} and E_{disp} in Tables 1, 2 and S3: Orange triangles, blue circles, red crosses, pink asterisks, and green squares indicate E_{int} calculated for thiophene-, furan-, pyrrole-, and pyridine-based heteroatom-PACs, respectively. Symbols of the same shape represent the respective compounds mentioned above, and the purple and green symbols correspond to E_{HF} and E_{disp}, respectively.

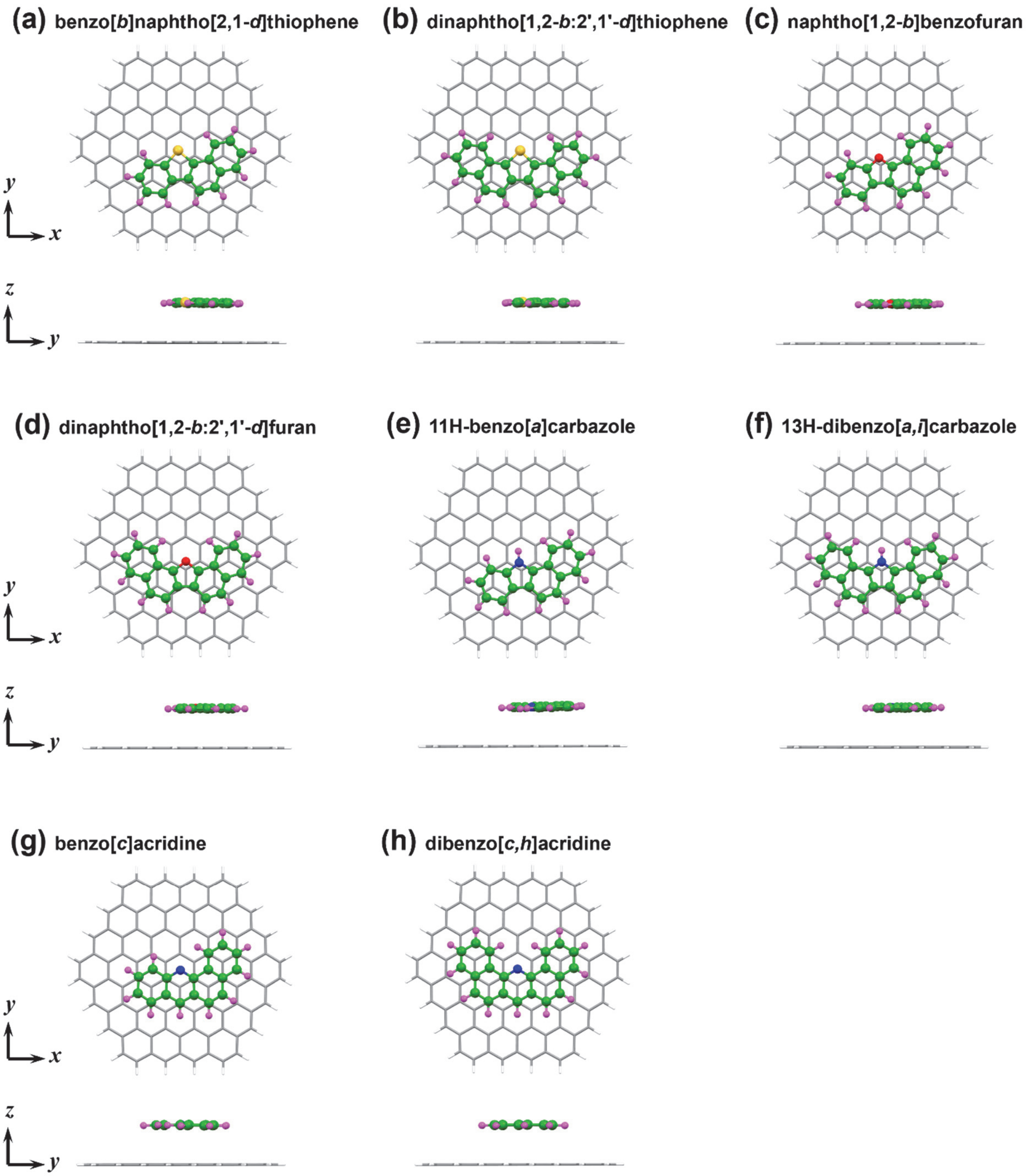


Fig. S4 Optimised geometries of $C_{96}H_{24}$ complexes with (a) benzo[*b*]naphtho[2,1-*d*]thiophene, (b) dinaphtho[1,2-*b*:2',1'-*d*]thiophene, (c) naphtho[1,2-*b*]benzofuran, (d) dinaphtho[1,2-*b*:2',1'-*d*]furan, (e) 11H-benzo[*a*]carbazole, (f) 13H-dibenzo[*a,i*]carbazole, (g) benzo[*c*]acridine and (h) dibenzo[*c,h*]acridine, viewed from different directions. The carbon, hydrogen, sulphur, oxygen and nitrogen atoms of adsorbed molecules are coloured in green, pink, yellow, red and blue, respectively.

Table S5 Interaction enegies calculated for $C_{96}H_{24}$ complexes with benzene-fused HACs and PAHs using the 6-311G** basis set, and contributions of dispersion forces.[a]

Adsorbate	Formula	E_{int} [b]	E_{HF} [c]	E_{disp} [d]	$E_{disp\text{-}corr}$ [e]
benzo[*b*]naphtho[2,1-*d*]thiophene	$C_{16}H_{10}S$	-27.29	14.58	-41.87	-38.56
naphtho[1,2-*b*]benzofuran	$C_{16}H_{10}O$	-25.23	13.48	-38.71	-35.80
11H-benzo[*a*]carbazole	$C_{16}H_{11}N$	-26.38	13.76	-40.14	-37.03
benzo[*c*]acridine	$C_{17}H_{11}N$	-28.07	14.91	-42.98	-39.81
dinaphtho[1,2-*b*:2',1'-*d*]thiophene	$C_{20}H_{12}S$	-32.76	17.69	-50.45	-46.40
dinaphtho[1,2-*b*:2',1'-*d*]furan	$C_{20}H_{12}O$	-30.88	16.65	-47.53	-43.86
13H-dibenzo[*a,i*]carbazole	$C_{20}H_{13}N$	-31.89	16.86	-48.75	-44.94
dibenzo[*c,h*]acridine	$C_{21}H_{13}N$	-33.89	18.04	-51.93	-48.10
phenanthrene [S2]	$C_{14}H_{10}$	-22.70	12.07	-34.77	-32.15
pyrene [S2]	$C_{16}H_{10}$	-25.23	13.12	-38.35	-35.52
tetracene [S2]	$C_{18}H_{12}$	-28.47	15.46	-43.93	-40.44
triphenylene [S2]	$C_{18}H_{12}$	-28.61	15.29	-43.90	-40.54
perylene [S2]	$C_{20}H_{12}$	-31.25	16.55	-47.80	-44.13
coronene [S2]	$C_{24}H_{12}$	-35.80	18.84	-54.64	-50.58

[a] Energy in kcal mol^{-1}.

[b] Interaction energy at B3LYP-D3/6-311G** level.

[c] Interaction energy at HF/6-311G** level.

[d] Dispersion energy estimated by the following equation: $E_{disp} = E_{int} - E_{HF}$.

[e] Dispersion-correction term in DFT calculations.

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6. Displaced geometries of $C_{96}H_{24}$ complexes with thiophene, furan, pyrrole and pyridine and change in interaction energies associated with horizontal displacement.

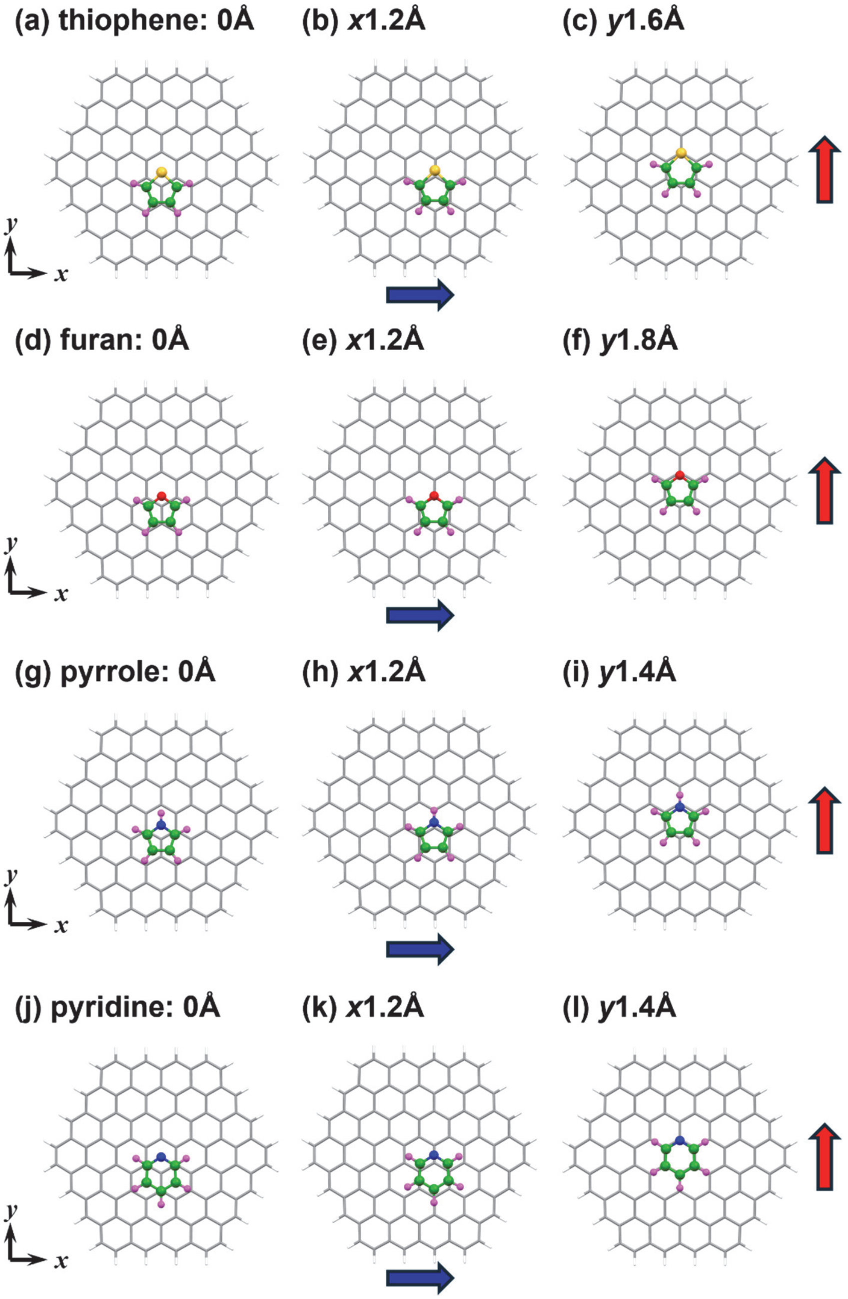


Fig. S5 The initial and displaced geometries of $C_{96}H_{24}$ complexes with (a-c) thiophene, (d-f) furan, (g-i) pyrrole and (j-l) pyridine. The adsorbates moved horizontally along the (b, e, h, k) *x*- or (c, f, I, l) *y*-axes at given distances from the initial position. The carbon, hydrogen, sulphur, oxygen and nitrogen atoms of adsorbed molecules are coloured in green, pink, yellow, red and blue, respectively.

Table S6 Interaction energy (E_{int}) and changes of E_{int} (ΔE_{int}) calculated for $C_{96}H_{24}$-thiophene complex associated with horizontal displacement at B3LYP-D3/6-311G** and HF/ 6-311G** levels. The plots of ΔE_{int} as a function of displacement are shown in Figs. 4(a,b) and S6.

Displacement / Å	***x***				***y***	
	B3LYP-D3/6-311G**		HF/ 6-311G**		B3LYP-D3/6-311G**	
	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]
0	-10.02	0	5.61	0	-10.02	0
0.2	-9.96	0.06	5.69	0.08	-10.00	0.02
0.4	-9.80	0.22	5.90	0.29	-9.88	0.14
0.6	-9.59	0.43	6.18	0.57	-9.68	0.34
0.8	-9.37	0.65	6.46	0.85	-9.44	0.58
1.0	-9.20	0.82	6.67	1.06	-9.19	0.83
1.2	-9.13	0.89	6.76	1.15	-8.99	1.03
1.4	-9.16	0.86	6.69	1.08	-8.88	1.14
1.6	-9.29	0.73	6.50	0.89	-8.87	1.15
1.8	-9.48	0.54	6.23	0.62	-8.96	1.06
2.0	-9.68	0.34	5.95	0.34	-9.10	0.92
2.2	-9.83	0.19	5.74	0.13	-9.27	0.75
2.4	-9.89	0.13	5.65	0.04	-9.41	0.61
2.6					-9.51	0.51
2.8					-9.57	0.45
3.0					-9.59	0.43
3.2					-9.60	0.42
3.4					-9.64	0.38
3.6					-9.70	0.32
3.8					-9.80	0.22
4.0					-9.88	0.14
4.2					-9.93	0.09

[a] Energy in kcal mol^{-1}.

Table S7 Interaction energy (E_{int}) and changes of E_{int} (ΔE_{int}) calculated for $C_{96}H_{24}$-furan complex associated with horizontal displacement at B3LYP-D3/6-311G** and HF/ 6-311G** levels. The plots of ΔE_{int} as a function of displacement are shown in Figs. 4(a,b) and S6.

Displacement / Å	***x***				***y***	
	B3LYP-D3/6-311G**		HF/ 6-311G**		B3LYP-D3/6-311G**	
	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]
0	-8.06	0	4.57	0	-8.06	0
0.2	-8.00	0.06	4.65	0.08	-8.06	0
0.4	-7.83	0.23	4.88	0.31	-8.00	0.06
0.6	-7.61	0.45	5.19	0.62	-7.88	0.18
0.8	-7.38	0.68	5.50	0.93	-7.70	0.36
1.0	-7.20	0.86	5.74	1.17	-7.50	0.56
1.2	-7.13	0.93	5.84	1.27	-7.30	0.76
1.4	-7.16	0.90	5.77	1.20	-7.15	0.91
1.6	-7.30	0.76	5.56	0.99	-7.08	0.98
1.8	-7.50	0.56	5.27	0.70	-7.08	0.98
2.0	-7.71	0.35	4.96	0.39	-7.15	0.91
2.2	-7.87	0.19	4.73	0.16	-7.27	0.79
2.4	-7.94	0.12	4.62	0.05	-7.41	0.65
2.6					-7.54	0.52
2.8					-7.65	0.41
3.0					-7.73	0.33
3.2					-7.78	0.28
3.4					-7.83	0.23
3.6					-7.88	0.18
3.8					-7.94	0.12
4.0					-8.00	0.06
4.2					-8.03	0.03

[a] Energy in kcal mol^{-1}.

Table S8 Interaction energy (E_{int}) and changes of E_{int} (ΔE_{int}) calculated for $C_{96}H_{24}$-pyrrole complex associated with horizontal displacement at B3LYP-D3/6-311G** and HF/ 6-311G** levels. The plots of ΔE_{int} as a function of displacement are shown in Figs. 4(a,b) and S6.

Displacement / Å	***x***				***y***	
	B3LYP-D3/6-311G**		HF/ 6-311G**		B3LYP-D3/6-311G**	
	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]
0	-9.02	0	4.58	0	-9.02	0
0.2	-8.97	0.05	4.65	0.07	-8.98	0.04
0.4	-8.83	0.19	4.87	0.29	-8.86	0.16
0.6	-8.63	0.39	5.15	0.57	-8.66	0.36
0.8	-8.43	0.59	5.45	0.87	-8.42	0.60
1.0	-8.27	0.75	5.67	1.09	-8.18	0.84
1.2	-8.21	0.81	5.75	1.17	-7.99	1.03
1.4	-8.24	0.78	5.69	1.11	-7.89	1.13
1.6	-8.37	0.65	5.49	0.91	-7.90	1.12
1.8	-8.55	0.47	5.21	0.63	-7.99	1.03
2.0	-8.73	0.29	4.92	0.34	-8.16	0.86
2.2	-8.87	0.15	4.70	0.12	-8.34	0.68
2.4	-8.93	0.09	4.60	0.02	-8.52	0.50
2.6					-8.65	0.37
2.8					-8.79	0.23
3.0					-8.78	0.24
3.2					-8.79	0.23
3.4					-8.81	0.21
3.6					-8.85	0.17
3.8					-8.90	0.12
4.0					-8.95	0.07
4.2					-8.97	0.05

[a] Energy in kcal mol^{-1}.

Table S9 Interaction energy (E_{int}) and changes of E_{int} (ΔE_{int}) calculated for $C_{96}H_{24}$-pyridine complex associated with horizontal displacement at B3LYP-D3/6-311G** and HF/ 6-311G** levels. The plots of ΔE_{int} as a function of displacement are shown in Figs. 4(a,b) and S6.

Displacement / Å	***x***				***y***	
	B3LYP-D3/6-311G**		HF/ 6-311G**		B3LYP-D3/6-311G**	
	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]
0	-10.14	0	4.89	0	-10.14	0
0.2	-10.10	0.04	4.95	0.06	-10.12	0.02
0.4	-10.00	0.14	5.10	0.21	-10.04	0.10
0.6	-9.87	0.27	5.31	0.42	-9.90	0.24
0.8	-9.73	0.41	5.51	0.62	-9.72	0.42
1.0	-9.63	0.51	5.67	0.78	-9.53	0.61
1.2	-9.58	0.56	5.73	0.84	-9.37	0.77
1.4	-9.60	0.54	5.68	0.79	-9.29	0.85
1.6	-9.67	0.47	5.54	0.65	-9.30	0.84
1.8	-9.78	0.36	5.35	0.46	-9.39	0.75
2.0	-9.90	0.24	5.15	0.26	-9.55	0.59
2.2	-9.98	0.16	5.00	0.11	-9.74	0.40
2.4	-10.00	0.14	4.94	0.05	-9.91	0.23
2.6					-10.04	0.10
2.8					-10.10	0.04
3.0					-10.12	0.02
3.2					-10.09	0.05
3.4					-10.06	0.08
3.6					-10.04	0.10
3.8					-10.05	0.09
4.0					-10.07	0.07
4.2					-10.07	0.07

[a] Energy in kcal mol^{-1}.

Table S10 Interaction energy (E_{int}) and changes of E_{int} (ΔE_{int}) calculated for $C_{96}H_{24}$-benzene complex associated with horizontal displacement at B3LYP-D3/6-311G** [S2] and HF/ 6-311G** levels. The plots of ΔE_{int} as a function of displacement are shown in Figs. 4(a,b) and S6.

Displacement / Å	***x***				***y***	
	B3LYP-D3/6-311G**		HF/ 6-311G**		B3LYP-D3/6-311G**	
	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]
0	-10.43	0	5.62	0	-10.43	0
0.2	-10.40	0.03	5.66	0.04	-10.40	0.03
0.4	-10.31	0.12	5.78	0.16	-10.30	0.13
0.6	-10.19	0.24	5.93	0.31	-10.13	0.3
0.8	-10.07	0.36	6.09	0.47	-9.92	0.51
1.0	-9.98	0.45	6.21	0.59	-9.72	0.71
1.2	-9.94	0.49	6.25	0.63	-9.56	0.87
1.4	-9.96	0.47	6.21	0.59	-9.50	0.93
1.6	-10.02	0.41	6.10	0.48	-9.54	0.89
1.8	-10.11	0.32	5.95	0.33	-9.67	0.76
2.0	-10.21	0.22	5.80	0.18	-9.87	0.56
2.2	-10.28	0.15	5.70	0.08	-10.09	0.34
2.4	-10.29	0.14	5.66	0.04	-10.27	0.16
2.6					-10.38	0.05
2.8					-10.43	0
3.0					-10.41	0.02
3.2					-10.35	0.08
3.4					-10.30	0.13
3.6					-10.27	0.16
3.8					-10.28	0.15
4.0					-10.29	0.14
4.2					-10.30	0.13

[a] Energy in kcal mol^{-1}.

S2 Y. Kikkawa and S. Tsuzuki, *Phys. Chem. Chem. Phys.*, 2025, **27**, 7421.

Table S11 Interaction energy (E_{int}) and changes of E_{int} (ΔE_{int}) calculated for $C_{96}H_{24}$-*n*-pentane complex associated with horizontal displacement at B3LYP-D3/6-311G** [S3] and HF/ 6-311G** levels. The plots of ΔE_{int} as a function of displacement are shown in Figs. 4(a,b) and S6.

Displacement / Å	***x***				***y***	
	B3LYP-D3/6-311G**		HF/ 6-311G**		B3LYP-D3/6-311G**	
	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]
0	-11.63	0	7.05	0	-11.63	0
0.2	-11.52	0.11	7.19	0.14	-11.54	0.09
0.4	-11.23	0.40	7.58	0.53	-11.24	0.39
0.6	-10.83	0.80	8.11	1.06	-10.82	0.81
0.8	-10.44	1.19	8.65	1.60	-10.39	1.24
1.0	-10.14	1.49	9.06	2.01	-10.05	1.58
1.2	-10.00	1.63	9.24	2.19	-9.86	1.77
1.4	-10.06	1.57	9.14	2.09	-9.81	1.82
1.6	-10.30	1.33	8.79	1.74	-9.86	1.77
1.8	-10.65	0.98	8.28	1.23	-9.95	1.68
2.0	-11.03	0.60	7.73	0.68	-10.02	1.61
2.2	-11.34	0.29	7.30	0.25	-10.03	1.60
2.4	-11.47	0.16	7.08	0.03	-9.99	1.64
2.6					-9.90	1.73
2.8					-9.81	1.82
3.0					-9.78	1.85
3.2					-9.88	1.75
3.4					-10.13	1.50
3.6					-10.51	1.12
3.8					-10.93	0.70
4.0					-11.28	0.35
4.2					-11.45	0.18

[a] Energy in kcal mol^{-1}.

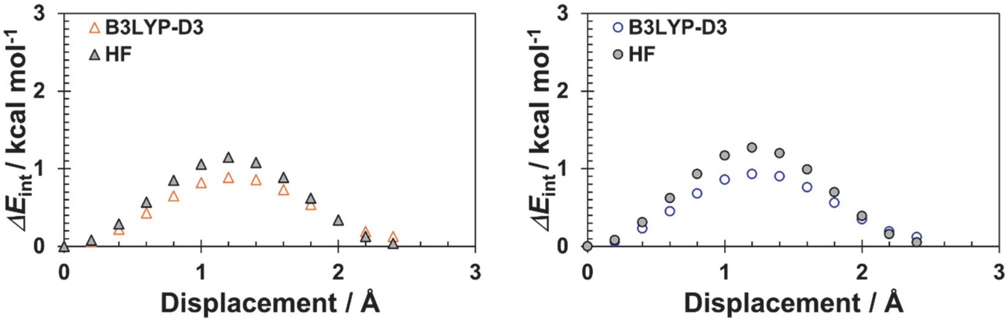
[S3] Y. Kikkawa and S. Tsuzuki, *Phys. Chem. Chem. Phys.*, 2024, **26**, 24314.

Table S12 Interaction energy (E_{int}) and changes of E_{int} (ΔE_{int}) calculated for $C_{96}H_{24}$-thiophene, $C_{96}H_{24}$-furan, $C_{96}H_{24}$-pyrrole, $C_{96}H_{24}$-pyridine and $C_{96}H_{24}$-benzene complexes associated with their rotation. The plots of ΔE_{int} as a function of the rotation are shown in Fig. Figs. 4(c).

Angle/ degree	thiophene		furan		pyrrole		pyridine		benzene	
	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]	E_{int} [a]	ΔE_{int} [a]
0	-10.02	0.01	-8.06	0.01	-9.02	0	-10.14	0.01	-10.43	0
10	-9.99	0.04	-8.04	0.03	-9.00	0.02	-10.11	0.04	-10.41	0.02
20	-9.92	0.11	-7.98	0.09	-8.93	0.09	-10.07	0.08	-10.37	0.06
30	-9.81	0.22	-7.88	0.19	-8.85	0.17	-10.04	0.11	-10.36	0.07
40	-9.69	0.34	-7.77	0.30	-8.77	0.25	-10.05	0.10	-10.37	0.06
50	-9.60	0.43	-7.67	0.40	-8.71	0.31	-10.07	0.08	-10.41	0.02
60	-9.57	0.46	-7.64	0.43	-8.68	0.34	-10.08	0.07	-10.43	0
70	-9.61	0.42	-7.68	0.39	-8.67	0.35	-10.07	0.08		
80	-9.70	0.33	-7.78	0.29	-8.69	0.33	-10.05	0.10		
90	-9.82	0.21	-7.90	0.17	-8.72	0.30	-10.05	0.10		
100	-9.93	0.10	-7.99	0.08	-8.75	0.27	-10.08	0.07		
110	-10.00	0.03	-8.05	0.02	-8.76	0.26	-10.13	0.02		
120	-10.03	0	-8.07	0	-8.76	0.26	-10.15	0		

[a] Energy in kcal mol^{-1}.

(a) thiophene (b) furan



(c) pyrrole (d) pyridine

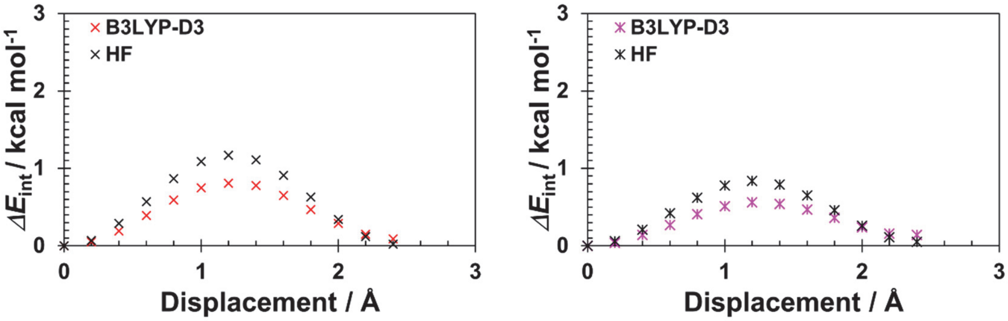


Fig. S6 Plots of changes of interaction energy (ΔE_{int}) calculated for $C_{96}H_{24}$ complexes with thiophene, furan, pyrrole and pyridine, associated with horizontal displacement along the *x*-axis. Black symbols denote the ΔE_{int} at HF level, whereas the coloured symbols denote those at B3LYP-D3 level.