Supporting Information

Assessment of Density Functional Theory in Predicting Interaction Energies Between Water and Polycyclic Aromatic Hydrocarbons: From Water on Benzene to Water on Graphene

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Contents

1 Geometries of polyciclic aromatic hydrocarbons

1.1 Benzene: C_6H_6

Table S1: Cartesian coordinates (in Å) of the ground-state geometries of the zero-, one-, and two-leg configurations of C_6H_6.

Structure	Atom	X	Y	Z
zero-leg	C	1.4222050	0.0014880	0.0000000
	C	0.7123920	1.2309210	0.0000000
	C	-0.7072350	1.2309210	0.0000000
	C	-1.4170480	0.0014880	0.0000000
	C	-0.7072350	-1.2279440	0.0000000
	C	0.7123920	-1.2279440	0.0000000
	H	1.2568920	-2.1710460	0.0000000
	H	-1.2517350	-2.1710450	0.0000000
	H	-2.5060480	0.0014880	0.0000000
	H	-1.2517350	2.1740230	0.0000000
	H	1.2568920	2.1740230	0.0000000
	H	2.5112050	0.0014880	0.0000000
one-leg	C	0.0000000	1.41962650	0.0000000
	C	1.2294330	0.70981350	0.0000000
	C	1.2294330	-0.70981350	0.0000000
	C	0.0000000	-1.41962650	0.0000000
	C	-1.2294320	-0.70981350	0.0000000
	C	-1.2294320	0.70981350	0.0000000
	H	-2.1725340	1.25431350	0.0000000
	H	-2.1725330	-1.25431350	0.0000000
	H	0.0000000	-2.50862650	0.0000000
	H	2.1725350	-1.25431350	0.0000000
	H	2.1725350	1.25431350	0.0000000
	H	0.0000000	2.50862650	0.0000000
two-leg	C	1.4222050	0.0014880	0.0000000
	C	0.7123920	1.2309210	0.0000000
	C	-0.7072350	1.2309210	0.0000000

Table S1 (continued).

Structure	Atom	X	Y	Z
	C	-1.4170480	0.0014880	0.0000000
	C	-0.7072350	-1.2279440	0.0000000
	C	0.7123920	-1.2279440	0.0000000
	H	1.2568920	-2.1710460	0.0000000
	H	-1.2517350	-2.1710450	0.0000000
	H	-2.5060480	0.0014880	0.0000000
	H	-1.2517350	2.1740230	0.0000000
	H	1.2568920	2.1740230	0.0000000
	H	2.5112050	0.0014880	0.0000000

1.2 Coronene: $C_{24}H_{12}$

1.2.1 Zero- and two-leg $C_{24}H_{12}$ configurations

Table S2: Cartesian coordinates (in Å) of the ground-state geometries of the zero- and two-leg configurations of $C_{24}H_{12}$.

Atom	X	Y	Z
C	2.8392528	-2.4588647	0.0000000
C	1.4196268	-2.4588647	0.0000000
C	0.7098128	-1.2294327	0.0000000
C	1.4196268	0.0000003	0.0000000
C	2.8392528	0.0000003	0.0000000
C	3.5490658	-1.2294327	0.0000000
C	3.5490658	1.2294323	0.0000000
C	2.8392528	2.4588653	0.0000000
C	1.4196268	2.4588653	0.0000000
C	0.7098128	1.2294323	0.0000000
C	-0.7098132	1.2294323	0.0000000
C	-1.4196262	2.4588653	0.0000000
C	-0.7098132	3.6882973	0.0000000
C	0.7098128	3.6882973	0.0000000
C	-1.4196262	0.0000003	0.0000000
C	-0.7098132	-1.2294327	0.0000000
C	-2.8392522	2.4588653	0.0000000
C	-3.5490662	1.2294323	0.0000000
C	-2.8392522	0.0000003	0.0000000
C	-3.5490662	-1.2294327	0.0000000

Table S2 (continued).

Atom	X	Y	Z
C	-2.8392522	-2.4588647	0.0000000
C	-1.4196262	-2.4588647	0.0000000
C	-0.7098132	-3.6882977	0.0000000
C	0.7098128	-3.6882987	0.0000000
H	4.6380658	1.2294323	0.0000000
H	3.3837528	3.4019663	0.0000000
H	4.6380658	-1.2294327	0.0000000
H	3.3837528	-3.4019667	0.0000000
H	1.2543118	-4.6313997	0.0000000
H	-1.2543142	-4.6313997	0.0000000
H	-3.3837522	-3.4019667	0.0000000
H	-4.6380662	-1.2294327	0.0000000
H	-4.6380652	1.2294313	0.0000000
H	-3.3837522	3.4019663	0.0000000
H	-1.2543132	4.6313993	0.0000000
H	1.2543118	4.6313993	0.0000000

1.2.2 One-leg $C_{24}H_{12}$ configuration

Table S3: Cartesian coordinates (in Å) of the ground-state geometry of the one-leg configuration of $C_{24}H_{12}$.

Atom	X	Y	Z
C	-2.4588647	2.8392528	0.0000000
C	-2.4588647	1.4196268	0.0000000
C	-1.2294327	0.7098128	0.0000000
C	0.0000003	1.4196268	0.0000000
C	0.0000003	2.8392528	0.0000000
C	-1.2294327	3.5490658	0.0000000
C	1.2294323	3.5490658	0.0000000
C	2.4588653	2.8392528	0.0000000
C	2.4588653	1.4196268	0.0000000
C	1.2294323	0.7098128	0.0000000
C	1.2294323	-0.7098132	0.0000000
C	2.4588653	-1.4196262	0.0000000
C	3.6882973	-0.7098132	0.0000000
C	3.6882973	0.7098128	0.0000000

Table S3 (continued).

Atom	X	Y	Z
C	0.0000003	-1.4196262	0.0000000
C	-1.2294327	-0.7098132	0.0000000
C	2.4588653	-2.8392522	0.0000000
C	1.2294323	-3.5490662	0.0000000
C	0.0000003	-2.8392522	0.0000000
C	-1.2294327	-3.5490662	0.0000000
C	-2.4588647	-2.8392522	0.0000000
C	-2.4588647	-1.4196262	0.0000000
C	-3.6882977	-0.7098132	0.0000000
C	-3.6882987	0.7098128	0.0000000
H	1.2294323	4.6380658	0.0000000
H	3.4019663	3.3837528	0.0000000
H	-1.2294327	4.6380658	0.0000000
H	-3.4019667	3.3837528	0.0000000
H	-4.6313997	1.2543118	0.0000000
H	-4.6313997	-1.2543142	0.0000000
H	-3.4019667	-3.3837522	0.0000000
H	-1.2294327	-4.6380662	0.0000000
H	1.2294313	-4.6380652	0.0000000
H	3.4019663	-3.3837522	0.0000000
H	4.6313993	-1.2543132	0.0000000
H	4.6313993	1.2543118	0.0000000

1.3 Circumcoronene: $C_{54}H_{18}$

1.3.1 Zero- and two-leg $C_{54}H_{18}$ configurations

Table S4: Cartesian coordinates (in Å) of the ground-state geometries of the zero- and two-leg configurations of $C_{54}H_{18}$.

Atom	X	Y	Z
C	0.70981208	-3.68829817	0.00000000
C	-0.70981292	-1.22943217	0.00000000
C	-0.70981292	1.22943283	0.00000000
C	-0.70981292	3.68829783	0.00000000
C	-0.70981292	6.14716283	0.00000000
C	0.70981308	-1.22943217	0.00000000
C	0.70981308	1.22943283	0.00000000
C	0.70981308	3.68829783	0.00000000
C	0.70981308	-6.14716417	0.00000000
C	-0.70981392	-3.68829717	0.00000000
C	-0.70981392	-6.14716317	0.00000000
C	0.70981508	6.14716283	0.00000000
C	-1.41962592	-0.00000017	0.00000000
C	-1.41962592	2.45886483	0.00000000
C	-1.41962592	4.91772983	0.00000000
C	1.41962608	-2.45886517	0.00000000
C	1.41962608	-4.91773117	0.00000000
C	-1.41962692	-2.45886517	0.00000000
C	1.41962708	-0.00000017	0.00000000
C	1.41962708	2.45886483	0.00000000
C	1.41962708	4.91772983	0.00000000
C	-1.41962792	-4.91773017	0.00000000
C	-2.83925192	-0.00000017	0.00000000
C	-2.83925192	2.45886483	0.00000000
C	-2.83925192	-2.45886517	0.00000000
C	-2.83925192	4.91772983	0.00000000
C	2.83925208	-2.45886617	0.00000000
C	2.83925208	-4.91773117	0.00000000
C	2.83925308	-0.00000017	0.00000000
C	2.83925308	2.45886383	0.00000000
C	2.83925308	4.91772983	0.00000000
C	-2.83925392	-4.91773017	0.00000000
C	3.54906508	-1.22943317	0.00000000

Table S4 (continued).

Atom	X	Y	Z
C	3.54906508	-3.68829817	0.00000000
C	-3.54906592	-1.22943217	0.00000000
C	-3.54906592	1.22943283	0.00000000
C	-3.54906592	3.68829883	0.00000000
C	3.54906608	1.22943183	0.00000000
C	3.54906608	3.68829683	0.00000000
C	-3.54906692	-3.68829617	0.00000000
C	-4.96869192	1.22943383	0.00000000
C	4.96869208	-3.68829717	0.00000000
C	-4.96869292	-1.22943117	0.00000000
C	-4.96869292	3.68829683	0.00000000
C	4.96869308	1.22943183	0.00000000
C	4.96869308	-1.22943317	0.00000000
C	4.96869308	3.68829883	0.00000000
C	-4.96869392	-3.68829617	0.00000000
C	-5.67850492	0.00000083	0.00000000
C	5.67850508	2.45886583	0.00000000
C	-5.67850592	-2.45886417	0.00000000
C	-5.67850592	2.45886683	0.00000000
C	5.67850608	-0.00000117	0.00000000
C	5.67850608	-2.45886517	0.00000000
H	-1.25431292	7.09026383	0.00000000
H	1.25431308	-7.09026517	0.00000000
H	-1.25431392	-7.09026517	0.00000000
H	1.25431508	7.09026383	0.00000000
H	-3.38375192	5.86083183	0.00000000
H	3.38375208	-5.86083217	0.00000000
H	-3.38375292	-5.86083117	0.00000000
H	3.38375308	5.86083083	0.00000000
H	5.51319308	-4.63139817	0.00000000
H	5.51319308	4.63139983	0.00000000
H	-5.51319392	-4.63139817	0.00000000
H	-5.51319392	4.63139883	0.00000000
H	-6.76750492	0.00000083	0.00000000
H	6.76750508	-0.00000117	0.00000000
H	6.76750508	2.45886683	0.00000000
H	-6.76750592	-2.45886417	0.00000000
H	-6.76750592	2.45886683	0.00000000
H	6.76750608	-2.45886517	0.00000000

1.3.2 One-leg $C_{54}H_{18}$ configuration

Table S5: Cartesian coordinates (in Å) of the ground-state geometry of one-leg configuration of $C_{54}H_{18}$.

Atom	X	Y	Z
C	-3.68829817	0.70981208	0.00000000
C	-1.22943217	-0.70981292	0.00000000
C	1.22943283	-0.70981292	0.00000000
C	3.68829783	-0.70981292	0.00000000
C	6.14716283	-0.70981292	0.00000000
C	-1.22943217	0.70981308	0.00000000
C	1.22943283	0.70981308	0.00000000
C	3.68829783	0.70981308	0.00000000
C	-6.14716417	0.70981308	0.00000000
C	-3.68829717	-0.70981392	0.00000000
C	-6.14716317	-0.70981392	0.00000000
C	6.14716283	0.70981508	0.00000000
C	-0.00000017	-1.41962592	0.00000000
C	2.45886483	-1.41962592	0.00000000
C	4.91772983	-1.41962592	0.00000000
C	-2.45886517	1.41962608	0.00000000
C	-4.91773117	1.41962608	0.00000000
C	-2.45886517	-1.41962692	0.00000000
C	-0.00000017	1.41962708	0.00000000
C	2.45886483	1.41962708	0.00000000
C	4.91772983	1.41962708	0.00000000
C	-4.91773017	-1.41962792	0.00000000
C	-0.00000017	-2.83925192	0.00000000
C	2.45886483	-2.83925192	0.00000000
C	-2.45886517	-2.83925192	0.00000000
C	4.91772983	-2.83925192	0.00000000
C	-2.45886617	2.83925208	0.00000000
C	-4.91773117	2.83925208	0.00000000
C	-0.00000017	2.83925308	0.00000000
C	2.45886383	2.83925308	0.00000000
C	4.91772983	2.83925308	0.00000000
C	-4.91773017	-2.83925392	0.00000000
C	-1.22943317	3.54906508	0.00000000
C	-3.68829817	3.54906508	0.00000000
C	-1.22943217	-3.54906592	0.00000000

Table S5 (continued).

Atom	X	Y	Z
C	1.22943283	-3.54906592	0.00000000
C	3.68829883	-3.54906592	0.00000000
C	1.22943183	3.54906608	0.00000000
C	3.68829683	3.54906608	0.00000000
C	-3.68829617	-3.54906692	0.00000000
C	1.22943383	-4.96869192	0.00000000
C	-3.68829717	4.96869208	0.00000000
C	-1.22943117	-4.96869292	0.00000000
C	3.68829683	-4.96869292	0.00000000
C	1.22943183	4.96869308	0.00000000
C	-1.22943317	4.96869308	0.00000000
C	3.68829883	4.96869308	0.00000000
C	-3.68829617	-4.96869392	0.00000000
C	0.00000083	-5.67850492	0.00000000
C	2.45886583	5.67850508	0.00000000
C	-2.45886417	-5.67850592	0.00000000
C	2.45886683	-5.67850592	0.00000000
C	-0.00000117	5.67850608	0.00000000
C	-2.45886517	5.67850608	0.00000000
H	7.09026383	-1.25431292	0.00000000
H	-7.09026517	1.25431308	0.00000000
H	-7.09026517	-1.25431392	0.00000000
H	7.09026383	1.25431508	0.00000000
H	5.86083183	-3.38375192	0.00000000
H	-5.86083217	3.38375208	0.00000000
H	-5.86083117	-3.38375292	0.00000000
H	5.86083083	3.38375308	0.00000000
H	-4.63139817	5.51319308	0.00000000
H	4.63139983	5.51319308	0.00000000
H	-4.63139817	-5.51319392	0.00000000
H	4.63139883	-5.51319392	0.00000000
H	0.00000083	-6.76750492	0.00000000
H	-0.00000117	6.76750508	0.00000000
H	2.45886683	6.76750508	0.00000000
H	-2.45886417	-6.76750592	0.00000000
H	2.45886683	-6.76750592	0.00000000
H	-2.45886517	6.76750608	0.00000000

1.4 Circumcircumcoronene: $C_{96}H_{24}$

1.4.1 Zero-, one-, and two-leg $C_{96}H_{24}$ configurations

Table S6: Cartesian coordinates (in Å) of the ground-state geometries of zero-, one-, and two-leg configurations of $C_{96}H_{24}$.

Atom	X	Y	Z
C	-7.807945	-3.688297	0.000000
C	-7.098132	-4.917730	0.000000
C	-7.807945	-1.229432	0.000000
C	-7.098132	-2.458865	0.000000
C	-7.807945	1.229432	0.000000
C	-7.098132	0.000000	0.000000
C	-7.807945	3.688297	0.000000
C	-7.098132	2.458865	0.000000
C	-5.678505	-4.917730	0.000000
C	-4.968692	-6.147162	0.000000
C	-5.678505	-2.458865	0.000000
C	-4.968692	-3.688297	0.000000
C	-5.678505	0.000000	0.000000
C	-4.968692	-1.229432	0.000000
C	-5.678505	2.458865	0.000000
C	-4.968692	1.229432	0.000000
C	-3.549066	-6.147162	0.000000
C	-2.839253	-7.376595	0.000000
C	-3.549066	-3.688297	0.000000
C	-2.839253	-4.917730	0.000000
C	-3.549066	-1.229432	0.000000
C	-2.839253	-2.458865	0.000000
C	-3.549066	1.229432	0.000000
C	-2.839253	0.000000	0.000000
C	-1.419626	-7.376595	0.000000
C	-0.709813	-8.606027	0.000000
C	-1.419626	-4.917730	0.000000
C	-0.709813	-6.147162	0.000000
C	-1.419626	-2.458865	0.000000
C	-0.709813	-3.688297	0.000000
C	-1.419626	0.000000	0.000000
C	-0.709813	-1.229432	0.000000
C	-7.098132	4.917730	0.000000
C	-5.678505	4.917730	0.000000

Table S6 (continued).

C	-4.968692	3.688297	0.000000
C	-4.968692	6.147162	0.000000
C	-3.549066	3.688297	0.000000
C	-2.839253	2.458865	0.000000
C	-3.549066	6.147162	0.000000
C	-2.839253	4.917730	0.000000
C	-2.839253	7.376595	0.000000
C	-1.419626	2.458865	0.000000
C	-0.709813	1.229432	0.000000
C	-1.419626	4.917730	0.000000
C	-0.709813	3.688297	0.000000
C	-1.419626	7.376595	0.000000
C	-0.709813	6.147162	0.000000
C	-0.709813	8.606027	0.000000
C	0.709813	-8.606027	0.000000
C	0.709813	-6.147162	0.000000
C	1.419626	-7.376595	0.000000
C	0.709813	-3.688297	0.000000
C	1.419626	-4.917730	0.000000
C	0.709813	-1.229432	0.000000
C	1.419626	-2.458865	0.000000
C	2.839253	-7.376595	0.000000
C	2.839253	-4.917730	0.000000
C	3.549066	-6.147162	0.000000
C	2.839253	-2.458865	0.000000
C	3.549066	-3.688297	0.000000
C	4.968692	-6.147162	0.000000
C	4.968692	-3.688297	0.000000
C	5.678505	-4.917730	0.000000
C	7.098132	-4.917730	0.000000
C	0.709813	1.229432	0.000000
C	1.419626	0.000000	0.000000
C	0.709813	3.688297	0.000000
C	1.419626	2.458865	0.000000
C	0.709813	6.147162	0.000000
C	1.419626	4.917730	0.000000
C	0.709813	8.606027	0.000000
C	1.419626	7.376595	0.000000
C	2.839253	0.000000	0.000000
C	3.549066	-1.229432	0.000000
C	2.839253	2.458865	0.000000
C	3.549066	1.229432	0.000000
C	2.839253	4.917730	0.000000

Table S6 (continued).

C	3.549066	3.688297	0.000000
C	2.839253	7.376595	0.000000
C	3.549066	6.147162	0.000000
C	4.968692	-1.229432	0.000000
C	5.678505	-2.458865	0.000000
C	4.968692	1.229432	0.000000
C	5.678505	0.000000	0.000000
C	4.968692	3.688297	0.000000
C	5.678505	2.458865	0.000000
C	4.968692	6.147162	0.000000
C	5.678505	4.917730	0.000000
C	7.098132	-2.458865	0.000000
C	7.807945	-3.688297	0.000000
C	7.098132	0.000000	0.000000
C	7.807945	-1.229432	0.000000
C	7.098132	2.458865	0.000000
C	7.807945	1.229432	0.000000
C	7.098132	4.917730	0.000000
C	7.807945	3.688297	0.000000
H	-8.896945	3.688297	0.000000
H	-1.254313	-9.549129	0.000000
H	-3.383753	-8.319696	0.000000
H	-5.513192	7.090264	0.000000
H	-8.896945	-1.229432	0.000000
H	-5.513192	-7.090264	0.000000
H	-7.642632	-5.860831	0.000000
H	-8.896945	1.229432	0.000000
H	-7.642632	5.860831	0.000000
H	-8.896945	-3.688297	0.000000
H	-3.383753	8.319696	0.000000
H	-1.254313	9.549129	0.000000
H	1.254313	-9.549129	0.000000
H	3.383753	-8.319696	0.000000
H	5.513192	-7.090264	0.000000
H	7.642632	-5.860831	0.000000
H	1.254313	9.549129	0.000000
H	3.383753	8.319696	0.000000
H	5.513192	7.090264	0.000000
H	8.896945	-3.688297	0.000000
H	8.896945	-1.229432	0.000000
H	8.896945	1.229432	0.000000
H	7.642632	5.860831	0.000000
H	8.896945	3.688297	0.000000

1.5 $C_{150}H_{30}$ geometry

1.5.1 Zero-, one-, and two-leg $C_{150}H_{30}$ configurations

Table S7: Cartesian coordinates (in Å) of the ground-state geometries of 0-, 1- and 2-leg configurations of $C_{150}H_{30}$.

Atom	X	Y	Z
C	-9.937384	-4.917730	0.000000
C	-9.227571	-6.147162	0.000000
C	-9.937384	-2.458865	0.000000
C	-9.227571	-3.688297	0.000000
C	-9.937384	-0.000000	0.000000
C	-9.227571	-1.229432	0.000000
C	-9.937384	2.458865	0.000000
C	-9.227571	1.229432	0.000000
C	-9.937384	4.917730	0.000000
C	-9.227571	3.688297	0.000000
C	-7.807945	-6.147162	0.000000
C	-7.098132	-7.376595	0.000000
C	-7.807945	-3.688297	0.000000
C	-7.098132	-4.917730	0.000000
C	-7.807945	-1.229432	0.000000
C	-7.098132	-2.458865	0.000000
C	-7.807945	1.229432	0.000000
C	-7.098132	-0.000000	0.000000
C	-7.807945	3.688297	0.000000
C	-7.098132	2.458865	0.000000
C	-5.678505	-7.376595	0.000000
C	-4.968692	-8.606027	0.000000
C	-5.678505	-4.917730	0.000000
C	-4.968692	-6.147162	0.000000
C	-5.678505	-2.458865	0.000000
C	-4.968692	-3.688297	0.000000
C	-5.678505	-0.000000	0.000000
C	-4.968692	-1.229432	0.000000
C	-5.678505	2.458865	0.000000
C	-4.968692	1.229432	0.000000
C	-3.549066	-8.606027	0.000000
C	-2.839253	-9.835460	0.000000
C	-3.549066	-6.147162	0.000000

Table S7 (continued).

C	-2.839253	-7.376595	0.000000
C	-3.549066	-3.688297	0.000000
C	-2.839253	-4.917730	0.000000
C	-3.549066	-1.229432	0.000000
C	-2.839253	-2.458865	0.000000
C	-3.549066	1.229432	0.000000
C	-2.839253	-0.000000	0.000000
C	-1.419626	-9.835460	0.000000
C	-0.709813	-11.064892	0.000000
C	-1.419626	-7.376595	0.000000
C	-0.709813	-8.606027	0.000000
C	-1.419626	-4.917730	0.000000
C	-0.709813	-6.147162	0.000000
C	-1.419626	-2.458865	0.000000
C	-0.709813	-3.688297	0.000000
C	-1.419626	-0.000000	0.000000
C	-0.709813	-1.229432	0.000000
C	0.709813	-11.064892	0.000000
C	0.709813	-8.606027	0.000000
C	1.419626	-9.835460	0.000000
C	0.709813	-6.147162	0.000000
C	1.419626	-7.376595	0.000000
C	0.709813	-3.688297	0.000000
C	1.419626	-4.917730	0.000000
C	0.709813	-1.229432	0.000000
C	1.419626	-2.458865	0.000000
C	-9.227571	6.147162	0.000000
C	-7.807945	6.147162	0.000000
C	-7.098132	4.917730	0.000000
C	-7.098132	7.376595	0.000000
C	-5.678505	4.917730	0.000000
C	-4.968692	3.688297	0.000000
C	-5.678505	7.376595	0.000000
C	-4.968692	6.147162	0.000000
C	-4.968692	8.606027	0.000000
C	-3.549066	3.688297	0.000000
C	-2.839253	2.458865	0.000000
C	-3.549066	6.147162	0.000000
C	-2.839253	4.917730	0.000000
C	-3.549066	8.606027	0.000000
C	-2.839253	7.376595	0.000000
C	-2.839253	9.835460	0.000000
C	-1.419626	2.458865	0.000000

Table S7 (continued).

C	-0.709813	1.229432	0.000000
C	-1.419626	4.917730	0.000000
C	-0.709813	3.688297	0.000000
C	-1.419626	7.376595	0.000000
C	-0.709813	6.147162	0.000000
C	-1.419626	9.835460	0.000000
C	-0.709813	8.606027	0.000000
C	-0.709813	11.064892	0.000000
C	0.709813	1.229432	0.000000
C	1.419626	-0.000000	0.000000
C	0.709813	3.688297	0.000000
C	1.419626	2.458865	0.000000
C	0.709813	6.147162	0.000000
C	1.419626	4.917730	0.000000
C	0.709813	8.606027	0.000000
C	1.419626	7.376595	0.000000
C	0.709813	11.064892	0.000000
C	1.419626	9.835460	0.000000
C	2.839253	-9.835460	0.000000
C	2.839253	-7.376595	0.000000
C	3.549066	-8.606027	0.000000
C	2.839253	-4.917730	0.000000
C	3.549066	-6.147162	0.000000
C	2.839253	-2.458865	0.000000
C	3.549066	-3.688297	0.000000
C	4.968692	-8.606027	0.000000
C	4.968692	-6.147162	0.000000
C	5.678505	-7.376595	0.000000
C	4.968692	-3.688297	0.000000
C	5.678505	-4.917730	0.000000
C	7.098132	-7.376595	0.000000
C	7.098132	-4.917730	0.000000
C	7.807945	-6.147162	0.000000
C	9.227571	-6.147162	0.000000
C	2.839253	-0.000000	0.000000
C	3.549066	-1.229432	0.000000
C	2.839253	2.458865	0.000000
C	3.549066	1.229432	0.000000
C	2.839253	4.917730	0.000000
C	3.549066	3.688297	0.000000
C	2.839253	7.376595	0.000000

Table S7 (continued).

C	3.549066	6.147162	0.000000
C	2.839253	9.835460	0.000000
C	3.549066	8.606027	0.000000
C	4.968692	-1.229432	0.000000
C	5.678505	-2.458865	0.000000
C	4.968692	1.229432	0.000000
C	5.678505	-0.000000	0.000000
C	4.968692	3.688297	0.000000
C	5.678505	2.458865	0.000000
C	4.968692	6.147162	0.000000
C	5.678505	4.917730	0.000000
C	4.968692	8.606027	0.000000
C	5.678505	7.376595	0.000000
C	7.098132	-2.458865	0.000000
C	7.807945	-3.688297	0.000000
C	7.098132	-0.000000	0.000000
C	7.807945	-1.229432	0.000000
C	7.098132	2.458865	0.000000
C	7.807945	1.229432	0.000000
C	7.098132	4.917730	0.000000
C	7.807945	3.688297	0.000000
C	7.098132	7.376595	0.000000
C	7.807945	6.147162	0.000000
C	9.227571	-3.688297	0.000000
C	9.937384	-4.917730	0.000000
C	9.227571	-1.229432	0.000000
C	9.937384	-2.458865	0.000000
C	9.227571	1.229432	0.000000
C	9.937384	-0.000000	0.000000
C	9.227571	3.688297	0.000000
C	9.937384	2.458865	0.000000
C	9.227571	6.147162	0.000000
C	9.937384	4.917730	0.000000
H	-5.513192	-9.549129	0.000000
H	-11.026384	-4.917730	0.000000
H	-3.383753	-10.778561	0.000000
H	-7.642632	-8.319696	0.000000
H	-11.026384	2.458865	0.000000
H	-9.772071	-7.090264	0.000000
H	-11.026384	4.917730	0.000000
H	-11.026384	-0.000000	0.000000
H	-11.026384	-2.458865	0.000000
H	-1.254313	-12.007994	0.000000

Table S7 (continued).

H	1.254313	-12.007994	0.000000
H	-9.772071	7.090264	0.000000
H	-7.642632	8.319696	0.000000
H	-5.513192	9.549129	0.000000
H	-3.383753	10.778561	0.000000
H	-1.254313	12.007994	0.000000
H	1.254313	12.007994	0.000000
H	3.383753	-10.778561	0.000000
H	5.513192	-9.549129	0.000000
H	7.642632	-8.319696	0.000000
H	9.772071	-7.090264	0.000000
H	3.383753	10.778561	0.000000
H	5.513192	9.549129	0.000000
H	7.642632	8.319696	0.000000
H	11.026384	-4.917730	0.000000
H	11.026384	-2.458865	0.000000
H	11.026384	-0.000000	0.000000
H	11.026384	2.458865	0.000000
H	9.772071	7.090264	0.000000
H	11.026384	4.917730	0.000000

1.6 $C_{216}H_{36}$ geometry

1.6.1 Zero-, one-, and two-leg $C_{216}H_{36}$ configurations

Table S8: Cartesian coordinates (in Å) of the ground-state geometries of 0-, 1- and 2-leg configurations of $C_{216}H_{36}$.

Atom	X	Y	Z
C	-12.066823	-6.147162	0.000000
C	-11.357010	-7.376595	0.000000
C	-12.066823	-3.688297	0.000000
C	-11.357010	-4.917730	0.000000
C	-12.066823	-1.229432	0.000000
C	-11.357010	-2.458865	0.000000
C	-12.066823	1.229432	0.000000
C	-11.357010	-0.000000	0.000000
C	-12.066823	3.688297	0.000000
C	-11.357010	2.458865	0.000000
C	-12.066823	6.147162	0.000000
C	-11.357010	4.917730	0.000000
C	-9.937384	-7.376595	0.000000
C	-9.227571	-8.606027	0.000000
C	-9.937384	-4.917730	0.000000
C	-9.227571	-6.147162	0.000000
C	-9.937384	-2.458865	0.000000
C	-9.227571	-3.688297	0.000000
C	-9.937384	-0.000000	0.000000
C	-9.227571	-1.229432	0.000000
C	-9.937384	2.458865	0.000000
C	-9.227571	1.229432	0.000000
C	-9.937384	4.917730	0.000000
C	-9.227571	3.688297	0.000000
C	-7.807945	-8.606027	0.000000
C	-7.098132	-9.835460	0.000000
C	-7.807945	-6.147162	0.000000
C	-7.098132	-7.376595	0.000000
C	-7.807945	-3.688297	0.000000
C	-7.098132	-4.917730	0.000000
C	-7.807945	-1.229432	0.000000
C	-7.098132	-2.458865	0.000000
C	-7.807945	1.229432	0.000000

Table S8 (continued).

Atom	X	Y	Z
C	-7.098132	-0.000000	0.000000
C	-7.807945	3.688297	0.000000
C	-7.098132	2.458865	0.000000
C	-5.678505	-9.835460	0.000000
C	-4.968692	-11.064892	0.000000
C	-5.678505	-7.376595	0.000000
C	-4.968692	-8.606027	0.000000
C	-5.678505	-4.917730	0.000000
C	-4.968692	-6.147162	0.000000
C	-5.678505	-2.458865	0.000000
C	-4.968692	-3.688297	0.000000
C	-5.678505	-0.000000	0.000000
C	-4.968692	-1.229432	0.000000
C	-5.678505	2.458865	0.000000
C	-4.968692	1.229432	0.000000
C	-3.549066	-11.064892	0.000000
C	-2.839253	-12.294324	0.000000
C	-3.549066	-8.606027	0.000000
C	-2.839253	-9.835460	0.000000
C	-3.549066	-6.147162	0.000000
C	-2.839253	-7.376595	0.000000
C	-3.549066	-3.688297	0.000000
C	-2.839253	-4.917730	0.000000
C	-3.549066	-1.229432	0.000000
C	-2.839253	-2.458865	0.000000
C	-3.549066	1.229432	0.000000
C	-2.839253	-0.000000	0.000000
C	-1.419626	-12.294324	0.000000
C	-0.709813	-13.523757	0.000000
C	-1.419626	-9.835460	0.000000
C	-0.709813	-11.064892	0.000000
C	-1.419626	-7.376595	0.000000
C	-0.709813	-8.606027	0.000000
C	-1.419626	-4.917730	0.000000
C	-0.709813	-6.147162	0.000000
C	-1.419626	-2.458865	0.000000
C	-0.709813	-3.688297	0.000000
C	-1.419626	-0.000000	0.000000
C	-0.709813	-1.229432	0.000000
C	0.709813	-13.523757	0.000000
C	0.709813	-11.064892	0.000000
C	1.419626	-12.294324	0.000000

Table S8 (continued).

Atom	X	Y	Z
C	0.709813	-8.606027	0.000000
C	1.419626	-9.835460	0.000000
C	0.709813	-6.147162	0.000000
C	1.419626	-7.376595	0.000000
C	0.709813	-3.688297	0.000000
C	1.419626	-4.917730	0.000000
C	0.709813	-1.229432	0.000000
C	1.419626	-2.458865	0.000000
C	-11.357010	7.376595	0.000000
C	-9.937384	7.376595	0.000000
C	-9.227571	6.147162	0.000000
C	-9.227571	8.606027	0.000000
C	-7.807945	6.147162	0.000000
C	-7.098132	4.917730	0.000000
C	-7.807945	8.606027	0.000000
C	-7.098132	7.376595	0.000000
C	-7.098132	9.835460	0.000000
C	-5.678505	4.917730	0.000000
C	-4.968692	3.688297	0.000000
C	-5.678505	7.376595	0.000000
C	-4.968692	6.147162	0.000000
C	-5.678505	9.835460	0.000000
C	-4.968692	8.606027	0.000000
C	-4.968692	11.064892	0.000000
C	-3.549066	3.688297	0.000000
C	-2.839253	2.458865	0.000000
C	-3.549066	6.147162	0.000000
C	-2.839253	4.917730	0.000000
C	-3.549066	8.606027	0.000000
C	-2.839253	7.376595	0.000000
C	-3.549066	11.064892	0.000000
C	-2.839253	9.835460	0.000000
C	-2.839253	12.294324	0.000000
C	-1.419626	2.458865	0.000000
C	-0.709813	1.229432	0.000000
C	-1.419626	4.917730	0.000000
C	-0.709813	3.688297	0.000000
C	-1.419626	7.376595	0.000000
C	-0.709813	6.147162	0.000000
C	-1.419626	9.835460	0.000000
C	-0.709813	8.606027	0.000000

Table S8 (continued).

Atom	X	Y	Z
C	-1.419626	12.294324	0.000000
C	-0.709813	11.064892	0.000000
C	-0.709813	13.523757	0.000000
C	0.709813	1.229432	0.000000
C	1.419626	-0.000000	0.000000
C	0.709813	3.688297	0.000000
C	1.419626	2.458865	0.000000
C	0.709813	6.147162	0.000000
C	1.419626	4.917730	0.000000
C	0.709813	8.606027	0.000000
C	1.419626	7.376595	0.000000
C	0.709813	11.064892	0.000000
C	1.419626	9.835460	0.000000
C	0.709813	13.523757	0.000000
C	1.419626	12.294324	0.000000
C	2.839253	-12.294324	0.000000
C	2.839253	-9.835460	0.000000
C	3.549066	-11.064892	0.000000
C	2.839253	-7.376595	0.000000
C	3.549066	-8.606027	0.000000
C	2.839253	-4.917730	0.000000
C	3.549066	-6.147162	0.000000
C	2.839253	-2.458865	0.000000
C	3.549066	-3.688297	0.000000
C	4.968692	-11.064892	0.000000
C	4.968692	-8.606027	0.000000
C	5.678505	-9.835460	0.000000
C	4.968692	-6.147162	0.000000
C	5.678505	-7.376595	0.000000
C	4.968692	-3.688297	0.000000
C	5.678505	-4.917730	0.000000
C	7.098132	-9.835460	0.000000
C	7.098132	-7.376595	0.000000
C	7.807945	-8.606027	0.000000
C	7.098132	-4.917730	0.000000
C	7.807945	-6.147162	0.000000
C	9.227571	-8.606027	0.000000
C	9.227571	-6.147162	0.000000
C	9.937384	-7.376595	0.000000
C	11.357010	-7.376595	0.000000
C	2.839253	-0.000000	0.000000
C	3.549066	-1.229432	0.000000

Table S8 (continued).

Atom	X	Y	Z
C	2.839253	2.458865	0.000000
C	3.549066	1.229432	0.000000
C	2.839253	4.917730	0.000000
C	3.549066	3.688297	0.000000
C	2.839253	7.376595	0.000000
C	3.549066	6.147162	0.000000
C	2.839253	9.835460	0.000000
C	3.549066	8.606027	0.000000
C	2.839253	12.294324	0.000000
C	3.549066	11.064892	0.000000
C	4.968692	-1.229432	0.000000
C	5.678505	-2.458865	0.000000
C	4.968692	1.229432	0.000000
C	5.678505	-0.000000	0.000000
C	4.968692	3.688297	0.000000
C	5.678505	2.458865	0.000000
C	4.968692	6.147162	0.000000
C	5.678505	4.917730	0.000000
C	4.968692	8.606027	0.000000
C	5.678505	7.376595	0.000000
C	4.968692	11.064892	0.000000
C	5.678505	9.835460	0.000000
C	7.098132	-2.458865	0.000000
C	7.807945	-3.688297	0.000000
C	7.098132	-0.000000	0.000000
C	7.807945	-1.229432	0.000000
C	7.098132	2.458865	0.000000
C	7.807945	1.229432	0.000000
C	7.098132	4.917730	0.000000
C	7.807945	3.688297	0.000000
C	7.098132	7.376595	0.000000
C	7.807945	6.147162	0.000000
C	7.098132	9.835460	0.000000
C	7.807945	8.606027	0.000000
C	9.227571	-3.688297	0.000000
C	9.937384	-4.917730	0.000000
C	9.227571	-1.229432	0.000000
C	9.937384	-2.458865	0.000000
C	9.227571	1.229432	0.000000
C	9.937384	-0.000000	0.000000

Table S8 (continued).

Atom	X	Y	Z
C	9.227571	3.688297	0.000000
C	9.937384	2.458865	0.000000
C	9.227571	6.147162	0.000000
C	9.937384	4.917730	0.000000
C	9.227571	8.606027	0.000000
C	9.937384	7.376595	0.000000
C	11.357010	-4.917730	0.000000
C	12.066823	-6.147162	0.000000
C	11.357010	-2.458865	0.000000
C	12.066823	-3.688297	0.000000
C	11.357010	-0.000000	0.000000
C	12.066823	-1.229432	0.000000
C	11.357010	2.458865	0.000000
C	12.066823	1.229432	0.000000
C	11.357010	4.917730	0.000000
C	12.066823	3.688297	0.000000
C	11.357010	7.376595	0.000000
C	12.066823	6.147162	0.000000
H	-13.155824	3.688297	0.000000
H	-13.155824	6.147162	0.000000
H	-13.155824	-6.147162	0.000000
H	-13.155824	-1.229432	0.000000
H	-9.772071	-9.549129	0.000000
H	-11.901510	-8.319696	0.000000
H	-13.155824	1.229432	0.000000
H	-13.155824	-3.688297	0.000000
H	-7.642632	-10.778561	0.000000
H	-5.513192	-12.007994	0.000000
H	-3.383753	-13.237426	0.000000
H	-1.254313	-14.466858	0.000000
H	1.254313	14.466858	0.000000
H	3.383753	-13.237426	0.000000
H	1.254313	-14.466858	0.000000
H	-11.901510	8.319696	0.000000
H	-9.772071	9.549129	0.000000
H	-7.642632	10.778561	0.000000
H	-5.513192	12.007994	0.000000
H	-3.383753	13.237426	0.000000

Table S8 (continued).

Atom	X	Y	Z
H	-1.254313	14.466858	0.000000
H	5.513192	-12.007994	0.000000
H	7.642632	-10.778561	0.000000
H	9.772071	-9.549129	0.000000
H	11.901510	-8.319696	0.000000
H	3.383753	13.237426	0.000000
H	5.513192	12.007994	0.000000
H	7.642632	10.778561	0.000000
H	9.772071	9.549129	0.000000
H	13.155824	-6.147162	0.000000
H	13.155824	-3.688297	0.000000
H	13.155824	-1.229432	0.000000
H	13.155824	1.229432	0.000000
H	13.155824	3.688297	0.000000
H	11.901510	8.319696	0.000000
H	13.155824	6.147162	0.000000

1.7 Water molecule geometry

1.7.1 Zero-leg configuration

Table S9: Cartesian coordinates (in Å) of the ground-state geometries of 0-leg configuration of water.

Atom	X	Y	Z
O	0.00000000	0.00000000	2.23659840
H	0.75659230	0.00000000	2.82294300
H	-0.75659230	0.00000000	2.82294300
O	0.00000000	0.00000000	2.51617320
H	0.75659230	0.00000000	3.10251780
H	-0.75659230	0.00000000	3.10251780
O	0.00000000	0.00000000	2.79574800
H	0.75659230	0.00000000	3.38209260
H	-0.75659230	0.00000000	3.38209260
O	0.00000000	0.00000000	3.07532280
H	0.75659230	0.00000000	3.66166740
H	-0.75659230	0.00000000	3.66166740
O	0.00000000	0.00000000	3.35489760
H	0.75659230	0.00000000	3.94124220
H	-0.75659230	0.00000000	3.94124220
O	0.00000000	0.00000000	4.19362200
H	0.75659230	0.00000000	4.77996660
H	-0.75659230	0.00000000	4.77996660
O	0.00000000	0.00000000	8.07532280
H	0.75659230	0.00000000	8.66166740
H	-0.75659230	0.00000000	8.66166740
O	0.00000000	0.00000000	6.15064560
H	0.75659230	0.00000000	6.73699020
H	-0.75659230	0.00000000	6.73699020
O	0.00000000	0.00000000	10.06469280
H	0.75659230	0.00000000	10.65103740
H	-0.75659230	0.00000000	10.65103740

1.7.2 One-leg configuration

Table S10: Cartesian coordinates (in Å) of the ground-state geometries of 1-leg configuration of water.

Atom	X	Y	Z
O	-1.05935500	-0.61159850	2.62811900
H	-1.12161100	-0.64757550	1.67382400
H	-0.24364300	-0.14065050	2.79744100
O	-1.05935500	-0.61159850	2.87811900
H	-1.12161100	-0.64757550	1.92382400
H	-0.24364300	-0.14065050	3.04744100
O	-1.05935500	-0.61159850	3.28927900
H	-1.12161100	-0.64757550	2.33498400
H	-0.24364300	-0.14065050	3.45860100
O	-1.05935500	-0.61159850	3.70043900
H	-1.12161100	-0.64757550	2.74614400
H	-0.24364300	-0.14065050	3.86976100
O	-1.05935500	-0.61159850	4.11159900
H	-1.12161100	-0.64757550	3.15730400
H	-0.24364300	-0.14065050	4.28092100
O	-1.05935500	-0.61159850	4.93391900
H	-1.12161100	-0.64757550	3.97962400
H	-0.24364300	-0.14065050	5.10324100
O	-1.05935500	-0.61159850	6.16739900
H	-1.12161100	-0.64757550	5.21310400
H	-0.24364300	-0.14065050	6.33672100
O	-1.05935500	-0.61159850	8.00000000
H	-1.12161100	-0.64757550	7.04570500
H	-0.24364300	-0.14065050	8.16932200

1.7.3 Two-leg configuration

Table S11: Cartesian coordinates (in Å) of the ground-state geometries of 2-leg configuration of water.

Atom	X	Y	Z
O	-0.00000000	0.00000000	2.50468080
H	0.75659200	-0.00000000	1.91833580
H	-0.75659200	0.00000000	1.91833580
O	-0.00000000	0.00000000	2.80468080
H	0.75659200	-0.00000000	2.21833580
H	-0.75659200	0.00000000	2.21833580
O	-0.00000000	0.00000000	3.15526590
H	0.75659200	-0.00000000	2.56892090
H	-0.75659200	0.00000000	2.56892090
O	-0.00000000	0.00000000	3.50585100
H	0.75659200	-0.00000000	2.91950600
H	-0.75659200	0.00000000	2.91950600
O	-0.00000000	0.00000000	3.85643610
H	0.75659200	-0.00000000	3.27009110
H	-0.75659200	0.00000000	3.27009110
O	-0.00000000	0.00000000	4.20702120
H	0.75659200	-0.00000000	3.62067620
H	-0.75659200	0.00000000	3.62067620
O	-0.00000000	0.00000000	5.25877650
H	0.75659200	-0.00000000	4.67243150
H	-0.75659200	0.00000000	4.67243150
O	-0.00000000	0.00000000	8.05877650
H	0.75659200	-0.00000000	7.47243150
H	-0.75659200	0.00000000	7.47243150

2 Interaction energies from DFT calculations

2.1 Benzene

Table S12: Interaction energies, in kcal/mol, of the 0-, 1-, and 2-leg H_2O–C_6H_6 dimers. Distances (R) given in Å are the z-coordinates of the oxygen of H_2O relative to the $x-y$ plane of the PAH.

	R	BLYP-D3	PBE-D3	revPBE-D3	rVV10	SCAN-D3	SCAN+rVV10	B97M-rV	B3LYP-D3	PBE0-D3	revPBE0-D3	ωB97M-V
zero-leg	2.236	16.512	15.572	16.571	15.016	14.374	14.208	14.499	16.277	15.571	16.362	14.993
	2.516	6.227	6.053	6.618	5.614	5.281	5.257	5.324	6.184	6.103	6.499	5.741
	2.795	2.202	2.165	2.720	1.860	1.723	1.804	1.744	2.298	2.342	2.673	2.105
	3.075	0.923	0.722	1.297	0.556	0.512	0.661	0.555	1.027	0.997	1.333	0.863
	3.354	0.620	0.248	0.746	0.219	0.199	0.386	0.270	0.645	0.541	0.848	0.523
	4.193	0.557	0.250	0.357	0.300	0.338	0.465	0.324	0.538	0.409	0.495	0.464
	6.150	0.222	0.218	0.207	0.209	0.246	0.255	0.215	0.245	0.255	0.249	0.249
	8.075	0.092	0.098	0.095	0.094	0.107	0.108	0.098	0.104	0.112	0.109	0.111
	10.064	0.043	0.046	0.044	0.044	0.050	0.050	0.046	0.048	0.052	0.051	0.052
one-leg	2.628	7.673	6.382	7.090	6.975	5.702	5.581	8.209	7.745	6.590	7.016	7.910
	2.878	0.210	-0.471	0.050	-0.180	-0.968	-0.958	0.665	0.187	-0.438	-0.172	0.345
	3.289	-3.083	-3.404	-3.108	-3.168	-3.637	-3.454	-2.798	-3.191	-3.426	-3.303	-2.946
	3.700	-2.825	-3.108	-2.899	-2.796	-3.150	-2.898	-2.647	-2.957	-3.128	-3.042	-2.724
	4.111	-1.923	-2.270	-2.073	-1.971	-2.251	-2.011	-1.916	-2.072	-2.283	-2.174	-1.990
	4.933	-0.822	-1.064	-1.003	-0.918	-1.058	-0.929	-0.939	-0.950	-1.104	-1.052	-1.002
	6.167	-0.335	-0.388	-0.381	-0.360	-0.397	-0.369	-0.373	-0.379	-0.419	-0.411	-0.408
	8.000	-0.122	-0.130	-0.127	-0.126	-0.137	-0.133	-0.373	-0.135	-0.144	-0.141	-0.143
	10.278	-0.044	-0.047	-0.045	-0.045	-0.050	-0.049	-0.046	-0.049	-0.052	-0.051	-0.052
two-leg	2.504	11.236	9.441	9.637	9.848	8.166	7.876	10.385	10.500	8.772	9.035	9.484
	2.804	0.237	-0.108	-0.418	0.012	-0.997	-1.144	0.235	0.011	-0.614	-0.888	-0.204
	3.155	-3.440	-3.336	-3.501	-3.095	-3.739	-3.694	-3.042	-3.410	-3.549	-3.859	-3.167
	3.505	-3.340	-3.489	-3.244	-3.119	-3.652	-3.424	-3.094	-3.365	-3.523	-3.522	-3.133
	3.856	-2.401	-2.831	-2.462	-2.439	-2.917	-2.597	-2.413	-2.576	-2.831	-2.646	-2.462
	4.207	-1.619	-2.102	-1.827	-1.777	-2.164	-1.860	-1.766	-1.850	-2.129	-1.942	-1.835
	5.258	-0.607	-0.799	-0.766	-0.706	-0.809	-0.715	-0.735	-0.714	-0.8403	-0.808	-0.787
	8.058	-0.125	-0.132	-0.129	-0.128	-0.139	-0.135	-0.130	-0.138	-0.146	-0.143	-0.144
	10.166	-0.050	-0.053	-0.051	-0.052	-0.056	-0.056	-0.053	-0.056	-0.059	-0.058	-0.059

2.2 Coronene

Table S13: Interaction energies, in kcal/mol, of the 0-, 1-, and 2-leg H_2O–$C_{24}H_{12}$ dimers. Distances (R) given in Å are the z-coordinates of the oxygen of H_2O relative to the $x-y$ plane of the PAH.

	R	BLYP-D3	PBE-D3	revPBE-D3	rVV10	SCAN-D3	SCAN+rVV10	B97M-rV	B3LYP-D3	PBE0-D3	revPBE0-D3	ωB97M-V
zero-leg	2.236	9.905	9.358	10.137	8.677	7.725	7.783	7.719	9.418	8.876	9.463	7.693
	2.516	1.755	1.861	2.302	1.290	0.8229	1.023	0.716	1.519	1.604	1.892	0.806
	2.795	-0.933	-0.780	-0.314	-1.200	-1.390	-1.092	-1.494	-0.992	-0.810	-0.536	-1.339
	3.075	-1.328	-1.395	-0.902	-1.658	-1.689	-1.349	-1.772	-1.340	-1.261	-0.965	-1.588
	3.354	-1.015	-1.283	-0.866	-1.393	-1.361	-1.018	-1.419	-1.068	-1.085	-0.815	-1.223
	4.193	-0.073	-0.293	-0.235	-0.292	-.177	0.018	-0.305	-0.095	-0.146	-0.085	-0.143
	8.075	0.145	0.1707	0.161	0.157	0.192	0.194	0.164	0.174	0.203	0.197	0.201
	6.150	0.228	-0.246	0.224	0.214	0.295	0.313	0.225	0.275	0.310	0.299	0.300
	10.064	0.093	-0.108	0.094	0.093	0.110	0.110	0.096	0.109	0.116	0.113	0.115
one-leg	2.628	7.149	6.611	6.797	7.089	5.978	6.047	8.158	7.531	6.883	6.878	7.904
	2.878	-0.204	-0.307	-0.161	-0.088	-0.741	-0.518	0.670	0.034	-0.191	-0.240	0.360
	3.289	-3.295	-3.323	-3.233	-3.080	-3.474	-3.064	-2.716	-3.273	-3.275	-3.320	-2.889
	3.700	-2.937	-3.114	-3.009	-2.756	-3.082	-2.617	-2.569	-3.023	-3.099	-3.085	-2.692
	4.111	-2.016	-2.357	-2.209	-2.005	-2.278	-1.866	-1.905	-2.167	-2.361	-2.275	-2.031
	4.933	-0.955	-1.228	-1.176	-1.058	-1.206	-0.991	-1.052	-1.111	-1.288	-1.230	-1.158
	6.167	-0.477	-0.558	-0.545	-0.521	-0.576	-0.524	-0.521	-0.547	-0.614	-0.596	-0.592
	8.000	-0.220	-0.246	-0.238	-0.237	-0.262	-0.255	-0.236	-0.249	-0.276	-0.268	-0.273
	10.278	-0.098	-0.108	-0.104	-0.105	-0.117	-0.116	-0.105	-0.110	-0.122	-0.119	-0.122
two-leg	2.504	8.380	7.456	7.107	7.941	6.448	6.489	8.359	8.096	7.034	6.834	7.657
	2.804	-1.103	-0.862	-1.487	-0.701	-1.573	-1.377	-0.534	-1.046	-1.195	-1.728	-0.845
	3.155	-4.022	-3.613	-3.948	-3.327	-3.890	-3.521	-3.263	-3.849	-3.722	-4.159	-3.350
	3.505	-3.649	-3.678	-3.535	-3.251	-3.743	-3.235	-3.177	-3.629	-3.664	-3.721	-3.236
	3.856	-2.631	-3.029	-2.731	-2.586	-3.042	-2.497	-2.506	-2.809	-3.022	-2.863	-2.599
	4.207	-1.836	-2.320	-2.093	-1.959	-2.330	-1.859	-1.905	-2.088	-2.362	-2.186	-2.021
	5.258	-0.822	-1.035	-1.003	-0.933	-1.043	-0.891	-0.939	-0.960	-1.109	-1.067	-1.037
	8.058	-0.225	-0.250	-0.243	-0.241	-0.269	-0.262	-0.243	-0.258	-0.286	-0.279	-0.283
	10.166	-0.106	-0.118	-0.114	-0.115	-0.129	-0.128	-0.116	-0.122	-0.136	-0.133	-0.136

2.3 Circumcoronene

Table S14: Interaction energies, in kcal/mol, of the 0-, 1-, and 2-leg H_2O–$C_{54}H_{18}$ dimers. Distances (R) given in Å are the z-coordinates of the oxygen of H_2O relative to the $x-y$ plane of the PAH.

	R	BLYP-D3	PBE-D3	revPBE-D3	rVV10	SCAN-D3	SCAN+rVV10	B97M-rV	B3LYP-D3	PBE0-D3	revPBE0-D3	ωB97M-V
zero-leg	2.236	9.537	8.893	9.708	8.152	7.207	7.290	7.212	9.096	8.479	9.108	7.733
	2.516	1.331	1.361	1.831	0.730	0.261	0.480	0.155	1.077	1.089	1.411	0.484
	2.795	-1.385	-1.290	-0.800	-1.765	-1.960	-1.648	-2.068	-1.485	-1.366	-1.063	-1.815
	3.075	-1.787	-1.896	-1.383	-2.206	-2.245	-1.893	-2.332	-1.846	-1.817	-1.497	-2.113
	3.354	-1.463	-1.761	-1.327	-1.909	-1.887	-1.533	-1.945	-1.561	-1.618	-1.327	-1.745
	4.193	-0.430	-0.655	-0.590	-0.668	-0.565	-0.359	-0.687	-0.481	-.545	-.473	-0.540
	8.075	0.143	0.183	0.171	0.164	0.209	0.212	0.168	0.179	0.222	0.214	0.215
	6.150	0.108	0.158	0.134	0.122	0.206	0.227	0.122	0.155	0.218	0.205	0.199
	10.064	0.109	0.133	0.126	0.123	0.1490	0.149	0.127	0.132	0.158	0.153	0.154
one-leg	2.628	6.859	6.478	6.647	6.861	5.963	6.103	7.982	7.336	6.854	6.854	7.867
	2.878	-0.406	-0.362	-0.239	-0.235	-0.687	-0.402	0.571	-0.085	-0.162	-0.212	0.357
	3.289	-3.365	-3.273	-3.204	-3.117	-3.335	-2.879	-2.712	-3.275	-3.156	-3.205	-2.813
	3.700	-2.921	-3.003	-2.917	-2.716	-2.901	-2.403	-2.495	-2.950	-2.932	-2.924	-2.558
	4.111	-1.953	-2.225	-2.092	-1.923	-2.091	-1.652	-1.793	-2.058	-2.183	-2.103	-1.871
	4.933	-0.873	-1.115	-1.073	-0.965	-1.061	-0.830	-0.940	-1.004	-1.151	-1.096	-1.021
	6.167	-0.432	-0.513	-0.5032	-0.480	-0.522	-0.463	-0.471	-0.497	-0.564	-0.548	-0.539
	8.000	-0.225	-0.260	-0.251	-0.250	-0.278	-0.270	-0.247	-0.259	-0.296	-0.288	-0.290
	10.278	-0.118	-0.138	-0.132	-0.132	-0.149	-0.149	-0.133	-0.137	-0.158	-0.154	-0.156
two-leg	2.504	8.189	7.390	7.063	7.778	6.493	6.597	8.290	8.043	7.133	6.966	7.888
	2.804	-1.191	-0.834	-1.470	-0.767	-1.453	-1.210	-0.548	-1.056	-1.087	-1.615	-0.760
	3.155	-4.033	-3.525	-3.873	-3.332	-3.727	-3.323	-3.228	-3.802	-3.576	-4.011	-3.268
	3.505	-3.610	-3.557	-3.427	-3.209	-3.560	-3.025	-3.103	-3.540	-3.493	-3.551	-3.120
	3.856	-2.564	-2.899	-2.612	-2.516	-2.861	-2.292	-2.406	-2.699	-2.850	-2.693	-2.459
	4.207	-1.758	-2.197	-1.979	-1.876	-2.165	-1.673	-1.796	-1.976	-2.205	-2.031	-1.879
	5.258	-0.764	-0.969	-0.942	-0.877	-0.960	-0.795	-0.869	-0.890	-1.032	-0.991	-0.957
	8.058	-0.257	-0.297	-0.287	-0.285	-0.319	-0.311	-0.284	-0.297	-0.340	-0.330	-0.333
	10.166	-0.143	-0.166	-0.160	-0.160	-0.181	-0.180	-0.161	-0.167	-0.191	-0.186	-0.189

3 Basis set error

3.1 GGA functionals

Table S15: Interaction energies, in kcal/mol, of the 0-, 1-, and 2-leg H_2O–C_6H_6 and H_2O–$C_{24}H_{12}$ dimers.

Molecule	R	BLYP-D3[a]	BLYP-D3[b]	PBE-D3[a]	PBE-D3[b]	revPBE-D3[a]	revPBE-D3[b]	rVV10[a]	rVV10[b]
Benzene	2.795	2.202	2.204	2.165	2.168	2.720	2.723	1.860	1.863
	3.075	0.923	0.931	0.722	0.729	1.297	1.304	0.556	0.563
	3.354	0.620	0.632	0.248	0.258	0.746	0.756	0.219	0.228
	2.878	0.210	0.186	-0.471	-0.490	0.050	0.034	-0.180	-0.199
	3.289	-3.083	-3.100	-3.404	-3.418	-3.108	-3.119	-3.168	-3.182
	3.700	-2.825	-2.834	-3.108	-3.116	-2.899	-2.906	-2.796	-2.805
	2.804	0.237	0.226	-0.108	-0.116	-0.418	-0.423	0.012	0.008
	3.155	-3.440	-3.451	-3.336	-3.347	-3.501	-3.508	-3.095	-3.103
	3.505	-3.340	-3.349	-3.489	-3.499	-3.244	-3.251	-3.119	-3.129
Coronene	2.795	-0.933	-1.004	-0.780	-0.849	-0.314	-0.358	-1.200	-1.275
	3.075	-1.328	-1.381	-1.395	-1.446	-0.902	-0.929	-1.658	-1.722
	3.354	-1.015	-1.057	-1.283	-1.323	-0.866	-0.882	-1.393	-1.449
	2.878	-0.204	-0.167	-0.307	-0.268	-0.161	-0.129	-0.088	-0.055
	3.289	-3.295	-3.255	-3.323	-3.283	-3.233	-3.197	-3.080	-3.044
	3.700	-2.937	-2.891	-3.114	-3.073	-3.009	-2.969	-2.756	-2.717
	2.804	-1.103	-1.037	-0.862	-0.800	-1.487	-1.438	-0.701	-0.635
	3.155	-4.022	-3.964	-3.613	-3.561	-3.948	-3.905	-3.327	-3.273
	3.505	-3.649	-3.596	-3.678	-3.631	-3.535	-3.492	-3.251	-3.205

[a] def2-QZVPPD basis applied on oxygen and hydrogen of H_2O and the six central carbon atoms of PAH, while the remaining atoms are treated with 6-31+G basis set.
[b] def2-QZVPPD basis set applied on all atoms.

3.2 meta-GGA functionals

Table S16: Interaction energies, in kcal/mol, of the 0-, 1-, and 2-leg H_2O–C_6H_6 and H_2O–$C_{24}H_{12}$ dimers.

Molecule	R	SCAN-D3[a]	SCAN-D3[b]	SCAN+rVV10[a]	SCAN+rVV10[b]	B97M-rV[a]	B97M-rV[b]
Benzene	2.795	1.723	1.720	1.804	1.802	1.744	1.742
	3.075	0.512	0.515	0.661	0.664	0.555	0.558
	3.354	0.199	0.202	0.386	0.390	0.270	0.277
	2.878	-0.968	-0.984	-0.958	-0.973	0.665	0.651
	3.289	-3.637	-3.648	-3.454	-3.465	-2.798	-2.808
	3.700	-3.150	-3.158	-2.898	-2.906	-2.647	-2.653
	2.804	-0.997	-1.004	-1.144	-1.152	0.235	0.237
	3.155	-3.739	-3.752	-3.694	-3.706	-3.042	-3.049
	3.505	-3.652	-3.665	-3.424	-3.438	-3.094	-3.105
Coronene	2.795	-1.390	-1.430	-1.092	-1.135	-1.494	-1.499
	3.075	-1.689	-1.727	-1.349	-1.389	-1.772	-1.777
	3.354	-1.361	-1.399	-1.018	-1.057	-1.419	-1.424
	2.878	-0.741	-0.757	-0.518	-0.535	0.670	0.623
	3.289	-3.474	-3.478	-3.064	-3.069	-2.716	-2.739
	3.700	-3.082	-3.079	-2.617	-2.616	-2.569	-2.575
	2.804	-1.573	-1.548	-1.377	-1.353	-0.534	-0.548
	3.155	-3.890	-3.879	-3.521	-3.511	-3.263	-3.274
	3.505	-3.743	-3.736	-3.235	-3.229	-3.177	-3.181

[a] def2-QZVPPD basis applied on oxygen and hydrogen of H_2O and the six central carbon atoms of PAH, while the remaining atoms are treated with 6-31+G basis set.
[b] def2-QZVPPD basis set applied on all atoms.

3.3 Hybrid functionals

Table S17: Interaction energies, in kcal/mol, of the 0-, 1-, and 2-leg H_2O–C_6H_6 and H_2O–$C_{24}H_{12}$ dimers.

Molecule	R	B3LYP-D3[a]	B3LYP-D3[b]	PBE0-D3[a]	PBE0-D3[b]	revPBE0-D3[a]	revPBE0-D3[b]	ωB97M-V[a]	ωB97M-V[b]
Benzene	2.795	2.298	2.303	2.342	2.348	2.673	2.678	2.105	2.100
	3.075	1.027	1.037	0.997	1.007	1.333	1.342	0.863	0.862
	3.354	0.645	0.657	0.541	0.551	0.848	0.859	0.523	0.522
	2.878	0.187	0.161	-0.438	-0.460	-0.172	-0.192	0.345	0.336
	3.289	-3.191	-3.210	-3.426	-3.441	-3.303	-3.317	-2.946	-2.952
	3.700	-2.957	-2.967	-3.128	-3.138	-3.042	-3.051	-2.724	-2.730
	2.804	0.011	-0.002	-0.614	-0.626	-0.888	-0.897	-0.204	-0.202
	3.155	-3.410	-3.424	-3.549	-3.562	-3.859	-3.871	-3.167	-3.175
	3.505	-3.365	-3.377	-3.523	-3.536	-3.522	-3.533	-3.133	-3.148
Coronene	2.795	-0.992	-1.034	-0.810	-0.838	-0.536	-0.543	-1.339	-1.357
	3.075	-1.340	-1.371	-1.261	-1.280	-0.965	-0.964	-1.588	-1.604
	3.354	-1.068	-1.092	-1.085	-1.100	-0.815	-0.810	-1.223	-1.242
	2.878	0.034	0.046	-0.191	-0.196	-0.240	-0.253	0.360	0.343
	3.289	-3.273	-3.254	-3.275	-3.271	-3.320	-3.321	-2.889	-2.897
	3.700	-3.023	-2.996	-3.099	-3.088	-3.085	-3.076	-2.692	-2.697
	2.804	-1.046	-1.004	-1.195	-1.176	-1.728	-1.721	-0.845	-0.839
	3.155	-3.849	-3.814	-3.722	-3.709	-4.159	-4.153	-3.350	-3.354
	3.505	-3.629	-3.595	-3.664	-3.650	-3.721	-3.710	-3.236	-3.242

[a] def2-QZVPPD basis applied on oxygen and hydrogen of H_2O and the six central carbon atoms of PAH, while the remaining atoms are treated with 6-31+G basis set.
[b] def2-QZVPPD basis set applied on all atoms.

4 Comparison between D3(0) and D3(BJ) damping models

To provide a balance treatment between the different dispersion flavors that exist, the more recent BJ-damping model[1] in the relevant density functional approximations is tested against the previous D3(0) variant,[2] as shown in Tables S18 and S19. In general, we observe that the choice of damping model can have a small effect on the interaction energy, within ∼0.2 kcal/mol in both 0- and 1-leg orientations of water and can be as large as 0.6 kcal/mol particularly for BLYP-D3 and revPBE0-D3 predictions of the 2-leg adsorption.

Table S18: Interaction energies, in kcal/mol, of the 0-, 1-, and 2-leg H_2O–C_6H_6, H_2O–$C_{24}H_{12}$, and H_2O–$C_{54}H_{18}$ dimers.

Molecule	R	BLYP-D3(0)	BLYP-D3(BJ)	PBE-D3(0)	PBE-D3(BJ)	revPBE-D3(0)	revPBE-D3(BJ)	SCAN-D3(0)	SCAN-D3(BJ)
Benzene	2.795	2.202	2.677	2.165	2.352	2.720	2.982	1.723	1.793
	3.075	0.923	1.174	0.722	0.900	0.875	1.287	0.512	0.625
	3.354	0.620	0.699	0.248	0.399	0.382	0.629	0.199	0.337
	2.878	0.210	0.328	-0.471	-0.485	-0.526	-0.039	-0.968	-1.038
	3.289	-3.083	-2.902	-3.404	-3.276	-3.306	-3.070	-3.637	-3.568
	3.700	-2.825	-2.658	-3.108	-2.955	-2.974	-2.877	-3.150	-3.020
	2.804	0.237	0.636	-0.108	-0.174	-0.227	-0.093	-0.997	-1.201
	3.155	-3.440	-2.815	-3.336	-3.160	-3.201	-3.043	-3.739	-3.802
	3.505	-3.340	-2.966	-3.489	-3.262	-3.291	-3.184	-3.652	-3.559
Coronene	2.795	-0.933	-0.543	-0.780	-0.516	-0.247	0.928	-1.390	-1.173
	3.075	-1.328	-1.579	-1.395	-1.150	-1.184	-1.068	-1.689	-1.447
	3.354	-1.015	-1.005	-1.283	-1.088	-1.112	-1.103	-1.361	-1.122
	2.878	-0.204	-0.073	-0.307	-0.229	-0.294	-0.422	-0.741	-0.712
	3.289	-3.295	-3.132	-3.323	-3.097	-3.144	-3.342	-3.474	-3.286
	3.700	-2.937	-2.807	-3.114	-2.888	-2.918	-3.116	-3.082	-2.838
	2.804	-1.103	-0.728	-0.862	-0.777	-0.853	-1.203	-1.573	-1.592
	3.155	-4.022	-3.461	-3.613	-3.319	-3.378	-3.710	-3.890	-3.770
	3.505	-3.649	-3.353	-3.678	-3.365	-3.406	-3.653	-3.743	-3.494
Circumcoronene	2.795	-1.385	-1.016	-1.290	-1.024	-0.800	-0.761	-1.960	-1.734
	3.075	-1.787	-1.634	-1.896	-1.684	-1.383	-1.572	-2.245	-1.996
	3.354	-1.463	-1.468	-1.761	-1.589	-1.327	-1.584	-1.887	-1.642
	2.878	-0.406	-0.309	-0.362	-0.340	-0.239	-0.549	-0.687	-0.625
	3.289	-3.365	-3.231	-3.273	-3.088	-3.204	-3.354	-3.335	-3.126
	3.700	-2.921	-2.812	-3.003	-2.805	-2.917	-3.055	-2.901	-2.644
	2.804	-1.191	-0.847	-0.834	-0.823	-1.470	-1.227	-1.453	-1.453
	3.155	-4.033	-3.499	-3.525	-3.288	-3.873	-3.669	-3.727	-3.594
	3.505	-3.610	-3.334	-3.557	-3.284	-3.427	-3.572	-3.560	-3.302

Table S19: Interaction energies, in kcal/mol, of the 0-, 1-, and 2-leg H_2O–C_6H_6, H_2O–$C_{24}H_{12}$, and H_2O–$C_{54}H_{18}$ dimers.

Molecule	R	B3LYP-D3(0)	B3LYP-D3(BJ)	PBE0-D3(0)	PBE0-D3(BJ)	revPBE0-D3(0)	revPBE0-D3(BJ)
Benzene	2.795	2.298	2.597	2.342	2.610	2.673	3.033
	3.075	1.027	1.148	0.997	1.134	1.333	1.436
	3.354	0.645	0.701	0.541	0.625	0.848	0.824
	2.878	0.187	0.111	-0.438	-0.351	-0.172	-0.131
	3.289	-3.191	-3.110	-3.426	-3.281	-3.303	-3.170
	3.700	-2.957	-2.832	-3.128	-2.987	-3.042	-2.934
	2.804	0.011	0.157	-0.614	-0.367	-0.888	-0.350
	3.155	-3.410	-3.138	-3.549	-3.299	-3.859	-3.293
	3.505	-3.365	-3.209	-3.523	-3.359	-3.522	-3.314
Coronene	2.795	-0.992	-0.687	-0.810	-0.511	-0.536	-0.294
	3.075	-1.340	-1.209	-1.261	-1.093	-0.965	-0.960
	3.354	-1.068	-1.005	-1.085	-0.979	-0.815	-0.917
	2.878	0.034	-0.044	-0.191	-0.065	-0.240	-0.260
	3.289	-3.273	-3.173	-3.275	-3.086	-3.320	-3.252
	3.700	-3.023	-2.881	-3.099	-2.921	-3.085	-3.045
	2.804	-1.046	-0.868	-1.195	-0.855	-1.728	-1.292
	3.155	-3.849	-3.562	-3.722	-3.423	-4.159	-3.715
	3.505	-3.629	-3.458	-3.664	-3.458	-3.721	-3.621
Circumcoronene	2.795	-1.485	-1.183	-1.366	-1.070	-1.063	-0.841
	3.075	-1.846	-1.717	-1.817	-1.652	-1.497	-1.509
	3.354	-1.561	-1.500	-1.618	-1.513	-1.327	-1.444
	2.878	-0.085	-0.164	-0.162	-0.032	-0.212	-0.267
	3.289	-3.275	-3.177	-3.156	-2.967	-3.205	-3.166
	3.700	-2.950	-2.810	-2.932	-2.755	-2.924	-2.904
	2.804	-1.056	-0.881	-1.087	-0.779	-1.615	-1.208
	3.155	-3.802	-3.518	-3.576	-3.279	-4.011	-3.591
	3.505	-3.540	-3.372	-3.493	-3.290	-3.551	-3.470

5 Comparison between hybrid and double-hybrid functionals

Due to the N^5 computational cost of DFT double hybrid approximations, we perform ωB97X-2(LP) and ωB97X-2(TQZ)[3] calculations, limiting ourselves to water–benzene and water–coronene interactions. The results obtained are summarized in Table S19. When compared to the data obtained from the hybrid functionals, the spread of the error is in the range 0.2–0.6, 0.1–0.3, and 0.1–0.8 kcal/mol for 0-, 1-, and 2-leg configurations, respectively.

Table S20: Interaction energies, in kcal/mol, of the 0-, 1-, and 2-leg H_2O–C_6H_6 and H_2O–$C_{24}H_{12}$ dimers.

Molecule	R	B3LYP-D3(0)	PBE0-D3(0)	revPBE0-D3(0)	ωB97M-V	ωB97X-2(LP)	ωB97X-2(TQZ)
Benzene	2.795	2.298	2.342	2.673	2.105	1.884	2.008
	3.075	1.027	0.997	1.333	0.863	0.606	0.656
	3.354	0.645	0.541	0.848	0.523	0.273	0.294
	2.878	0.187	-0.438	-0.172	0.345	-0.117	0.185
	3.289	-3.191	-3.426	-3.303	-2.946	-3.276	-3.145
	3.700	-2.957	-3.128	-3.042	-2.724	-2.991	-2.937
	2.804	0.011	-0.614	-0.888	-0.204	-0.480	-0.092
	3.155	-3.410	-3.549	-3.859	-3.167	-3.443	-3.274
	3.505	-3.365	-3.523	-3.522	-3.133	-3.450	-3.380
Coronene	2.795	-0.992	-0.810	-0.536	-1.339	-1.029	-0.880
	3.075	-1.340	-1.261	-0.965	-1.588	-1.403	-1.333
	3.354	-1.068	-1.085	-0.815	-1.223	-1.128	-1.084
	2.878	0.034	-0.191	-0.240	0.360	-0.194	0.199
	3.289	-3.273	-3.275	-3.320	-2.889	-3.256	-3.062
	3.700	-3.023	-3.099	-3.085	-2.692	-2.969	-2.868
	2.804	-1.046	-1.195	-1.728	-0.845	-1.140	-0.685
	3.155	-3.849	-3.722	-4.159	-3.350	-3.623	-3.396
	3.505	-3.629	-3.664	-3.721	-3.236	-3.528	-3.408

6 Comparisons with L-CCSD(T) and RPA values reported in the literature.

Fig. S1 and S2 show the comparison between the reference data obtained in this work and the results taken from Ref. 4. As discussed in Section 2.4 of manuscript, the L-CCSD(T) data calculated in this study employed the standard extrapolation scheme.[5,6] The corresponding numbers taken from Ref. 4 adopts a multiplicative procedure.

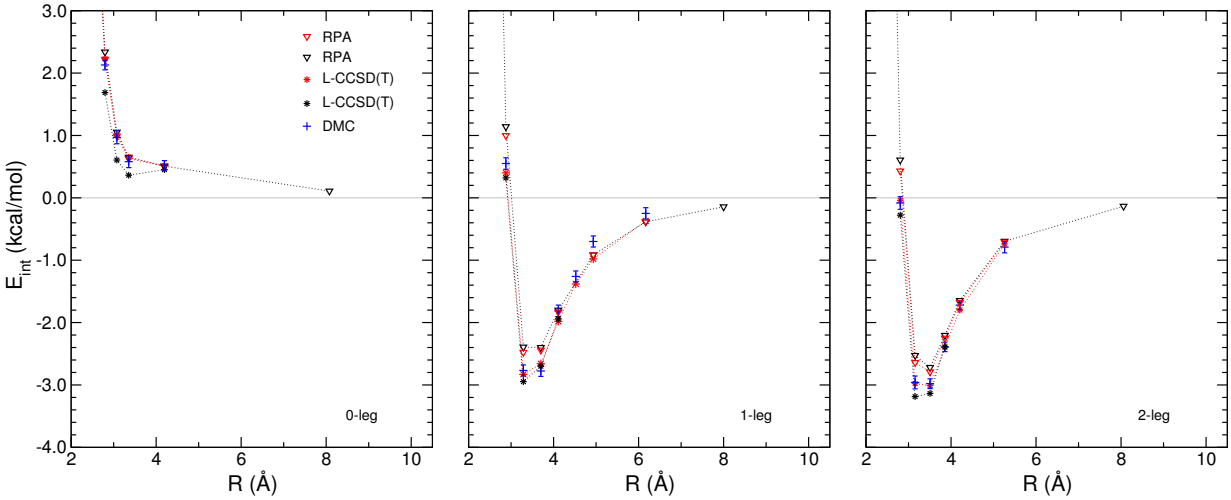

Figure S1: a) 0-, 1-, and 2-leg water–benzene data represented by black symbols are obtained in this work. b) 0-, 1-, and 2-leg water–benzene data represented by red symbols including DMC values are taken from Ref. 4.

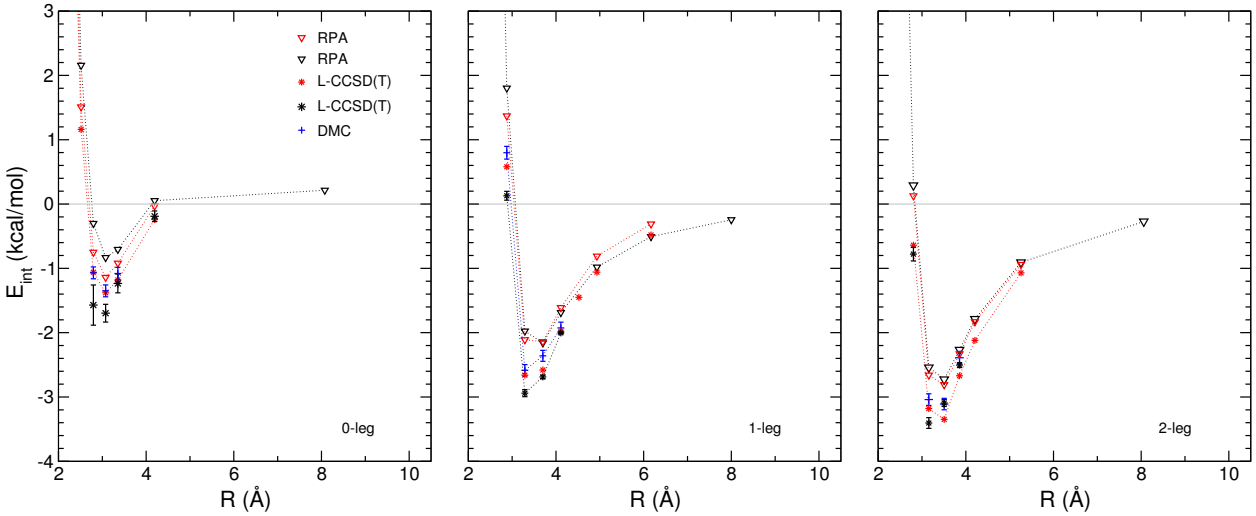

Figure S2: a) 0-, 1-, and 2-leg water–coronene data represented by black symbols are obtained in this work. b) 0-, 1-, and 2-leg water–coronene data represented by red symbols including DMC values are taken from Ref. 4.

7 L-CCSD(T) convergence with respect to basis sets and PNO thresholds.

Table S21: Comparison between the thresholds controlling L-CCSD(T) by calculating the interaction energies, in kcal/mol, of H_2O–C_6H_6 and H_2O–$C_{24}H_{12}$ dimers for the 0-, 1-, and 2-leg water configurations determined at 3.075, 3.289, and 3.155 Å, respectively.

	Structure	PNO threshold	Basis set			
			TZ	QZ	5Z	(Q,5)
Benzene	0-leg	Loose	1.686	1.284	1.015	0.734
		Normal	1.512	1.068	0.842	0.605
		Tight	1.791	1.360	1.079	0.785
	1-leg	Loose	-1.991	-2.372	-2.511	-2.657
		Normal	-2.206	-2.602	-2.770	-2.946
		Tight	-2.097	-2.503	-2.681	-2.868
	2-leg	Loose	-1.863	2.392	-2.588	-2.793
		Normal	-2.171	-2.710	-2.942	-3.186
		Tight	-1.953	-2.521	-2.760	-3.011
	CCSD(T)[a]		1.746[b]			0.591[e]
			-2.164[c]			-
			-2.057[d]			-3.171[f]
Coronene	0-leg	Loose	-0.755			
		Normal	-0.961			
		Tight	-0.717			
	1-leg	Loose	-1.927			
		Normal	-2.217			
		Tight	-2.005			
	2-leg	Loose	-2.174			
		Normal	-2.424			
		Tight	-2.196			

[a] Canonical CCSD(T) method. [b] CCSD(T) result for 0-leg water–benzene dimer. [c] CCSD(T) result for 1-leg water–benzene dimer. [d] CCSD(T) result for 2-leg water–benzene dimer. [e] CCSD(T)/CBS result for 0-leg water–benzene dimer taken from Ref. 7, where the vertical distance between the oxygen of water and the $x-y$ plane of benzene is 3.10 Å. [f] CCSD(T)/CBS result for 2-leg water–benzene dimer taken from Ref. 7, where the vertical distance between the oxygen of water and the $x-y$ plane of benzene is 3.20 Å.

Table S22: CPU timings corresponding to the thresholds controlling L-CCSD(T) involving H_2O–C_6H_6 and H_2O–$C_{24}H_{12}$ interactions.

	Structure	PNO Threshold	CPU Time (*min.*)		
			TZ	QZ	5Z
Benzene	0-leg	Loose	4	14	93
		Normal	6	27	131
		Tight	16	61	252
	1-leg	Loose	4	18	80
		Normal	6	28	130
		Tight	19	63	224
	2-leg	Loose	4	16	84
		Normal	7	31	139
		Tight	16	61	240
Coronene	0-leg	Loose	46		
		Normal	302		
		Tight	1490		
	1-leg	Loose	45		
		Normal	304		
		Tight	1549		
	2-leg	Loose	48		
		Normal	309		
		Tight	1547		

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