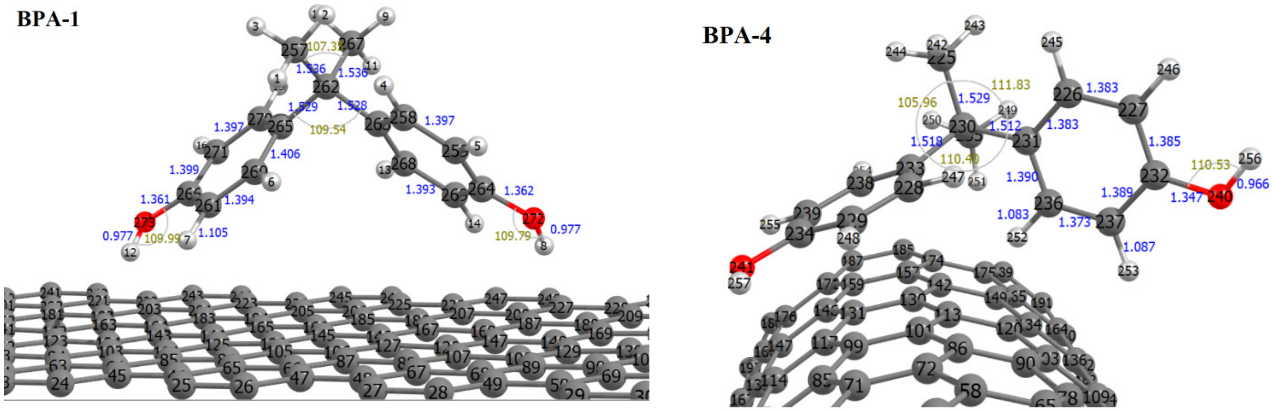
Supplementary material

Table S1. Covalent bond length between aliphatic and aromatic carbon atoms in Bisphenol A and its derivatives adsorbed on graphene surface.

Model	Method	C1-C2, Å	C2-C3, Å	C1-C2-C3, °
BPA	experiment [30]	1.536	1.536	109.2
PBA	CA	1.523	1.524	110.3
PBA	BH	1.530	1.531	110.0
PBA	PBE	1.540	1.540	110.7
PBA	DFT-D2	1.531	1.531	110.0
BPA-1	BH	1.529	1.528	109.5
BPA-2	BH	1.533	1.533	107.5
BPA-3	BH	1.530	1.533	108.9
DEBA	experiment [31]	1.528	1.548	108.4
DEBA	CA	1.526	1.522	108.7
DEBA	BH	1.529	1.530	108.6
DEBA	PBE	1.547	1.547	109.0
DEBA	DFT-D2	1.544	1.544	108.7
DEBA-GN	BH	1.531	1.531	108.7



a b

Fig. S1. (Color online) Examples of structural models with end-to-end numbering of atoms.

Table S2. Bond length in Bisphenol A molecules adsorbed on graphene surface (BH functional).

Model	Bond A1-A2	Number of Atom 1	Number of Atom 2	Bond length, Å
BPA-1	OH	273	12	0.9771
BPA-1	OH	272	8	0.9772
BPA-1	CH	270	15	1.1021
BPA-1	CH	258	4	1.1023
BPA-1	CH	271	16	1.1027
BPA-1	CH	269	14	1.1040
BPA-1	CH	261	7	1.1046
BPA-1	CH	268	13	1.1051
BPA-1	CH	260	6	1.1052
BPA-1	CH	267	11	1.1087
BPA-1	CH	257	3	1.1095
BPA-1	CH	257	2	1.1100
BPA-1	CH	267	10	1.1103
BPA-1	OC	273	266	1.3609
BPA-1	OC	272	264	1.3616
BPA-1	CC	268	269	1.3933
BPA-1	CC	260	261	1.3935
BPA-1	CC	270	271	1.3968

BPA-1	CC	266	271	1.3990
BPA-1	CC	259	264	1.3991
BPA-1	CC	265	270	1.4026
BPA-1	CC	258	263	1.4028
BPA-1	CC	261	266	1.4041
BPA-1	CC	263	268	1.4054
BPA-1	CC	260	265	1.4060
BPA-1	CC	262	263	1.5284
BPA-1	CC	262	265	1.5288
BPA-1	CC	262	267	1.5360
BPA-1	CC	257	262	1.5364
BPA-2	OH	273	16	0.9731
BPA-2	OH	272	5	0.9757
BPA-2	CH	265	9	1.1014
BPA-2	CH	271	15	1.1024
BPA-2	CH	269	14	1.1033
BPA-2	CH	257	1	1.1046
BPA-2	CH	262	7	1.1058
BPA-2	CH	257	3	1.1084
BPA-2	CH	266	12	1.1091
BPA-2	CH	257	2	1.1100
BPA-2	OC	272	260	1.3624
BPA-2	OC	273	270	1.3631
BPA-2	CC	269	271	1.3908
BPA-2	CC	258	259	1.3930
BPA-2	CC	268	270	1.3987
BPA-2	CC	260	262	1.3992
BPA-2	CC	265	267	1.4005
BPA-2	CC	270	271	1.4021
BPA-2	CC	258	260	1.4027
BPA-2	CC	261	264	1.4040
BPA-2	CC	267	269	1.4066
BPA-2	CC	259	261	1.4086
BPA-2	CC	267	266	1.5327
BPA-2	CC	261	263	1.5328
BPA-2	CC	257	263	1.5327
BPA-2	CC	263	266	1.5364
BPA-3	OH	272	8	0.9758
BPA-3	OH	273	12	0.9773
BPA-3	CH	261	7	1.1003
BPA-3	CH	270	15	1.1015
BPA-3	CH	271	16	1.1024
BPA-3	CH	258	4	1.1031
BPA-3	CH	269	14	1.1034
BPA-3	CH	268	13	1.1040
BPA-3	CH	259	5	1.1062
BPA-3	CH	267	11	1.1083
BPA-3	CH	257	1	1.1087
BPA-3	CH	257	3	1.1094
BPA-3	CH	267	9	1.1096
BPA-3	CH	267	10	1.1109
BPA-3	OC	273	266	1.3615
BPA-3	OC	272	264	1.3622
BPA-3	CC	268	269	1.3917
BPA-3	CC	260	261	1.3922
BPA-3	CC	270	271	1.3976
BPA-3	CC	259	264	1.3993

BPA-3	CC	266	271	1.3996
BPA-3	CC	261	266	1.4006
BPA-3	CC	258	263	1.4022
BPA-3	CC	264	269	1.4032
BPA-3	CC	265	270	1.4047
BPA-3	CC	263	268	1.4086
BPA-3	CC	262	265	1.5296
BPA-3	CC	262	263	1.5335
BPA-3	CC	257	262	1.5343
BPA-3	CC	262	267	1.5375
BPA-4	OH	240	256	0.9661
BPA-4	OH	241	257	0.9695
BPA-4	CH	236	252	1.0832
BPA-4	CH	226	245	1.0846
BPA-4	CH	238	254	1.0867
BPA-4	CH	237	253	1.0872
BPA-4	CH	228	247	1.0879
BPA-4	CH	229	248	1.0890
BPA-4	CH	225	244	1.0944
BPA-4	CH	235	249	1.0948
BPA-4	CH	235	250	1.0954
BPA-4	CH	235	251	1.0958
BPA-4	OC	240	232	1.3470
BPA-4	OC	241	234	1.3483
BPA-4	CC	236	237	1.3730
BPA-4	CC	238	239	1.3780
BPA-4	CC	228	229	1.3817
BPA-4	CC	226	231	1.3833
BPA-4	CC	227	232	1.3846
BPA-4	CC	229	234	1.3875
BPA-4	CC	234	239	1.3880
BPA-4	CC	232	237	1.3888
BPA-4	CC	228	233	1.3893
BPA-4	CC	233	238	1.3896
BPA-4	CC	231	236	1.3901
BPA-4	CC	230	231	1.5119
BPA-4	CC	230	233	1.5181
BPA-4	CC	225	230	1.5294
BPA-4	CC	230	235	1.5329

Table S3. Energy of formation, ΔE_{form}, for the different equilibrium configurations (DFT-D2).

Model	ΔE_{form}, kcal/mol
BPA-GN-1	−14.6
BPA-GN-2	−14.5
BPA-GN-3	−15.0
BPA-SWNT(7,7)	−29.7
DEBA-SWNT(7,7)	−16.5
DEBA-GN	−36.1

Table S4. Bond critical points of electron density calculated using Critic2 for Bisphenol A derivatives adsorbed on nanotubes and graphene.

Name of system	Bond	Bond type	$\rho(r_{bcp})$, a.u.	$\nabla^2\rho(r_{bcp})$, a.u.
BPA1	H12-C103	Cg...H-O	0.0135	0.046
BPA1	H8-C148	Cg...H-O	0.0147	0.047
BPA1	H7-C85	Cg...H	0.0071	0.024
BPA1	H14-C168	Cg...H	0.0078	0.026

BPA2	O272-C108	Cg...O	0.0066	0.026
BPA2	H1-C126	Cg...H	0.0107	0.035
BPA2	H10-C166	Cg...H	0.0076	0.026
BPA2	H7-C168	Cg...H	0.0063	0.024
BPA2	H5-C148	Cg...H	0.0080	0.027
BPA2	C258-C106	Cg…C	0.0037	0.011
BPA2	C264-C146	Cg…C	0.0055	0.020
BPA2	C260-C128	Cg…C	0.0075	0.027
BPA3	O272-C169	Cg...O	0.0102	0.036
BPA3	H12-C85	Cg...H	0.0109	0.036
BPA3	H7-C65	Cg...H	0.0126	0.040
BPA3	H6-C88	Cg...H	0.0035	0.011
BPA3	C264-C148	Cg…C	0.0048	0.017
BPA4	O241-C85	Cg...O	0.0159	0.057
BPA4	C142-H251	Cg...H	0.0045	0.014
BPA4	C120-H252	Cg...H	0.0168	0.057
BPA4	C103-H253	Cg...H	0.0092	0.034
BPA4	C99-C234	Cg…C	0.0166	0.043
BPA4	C71-C229	Cg…C	0.0105	0.028
DEBA-SWNT(5,5)	C116-O207	Cg...O	0.0100	0.038
DEBA-SWNT(5,5)	O206-C114	Cg...O	0.0181	0.078
DEBA-SWNT(5,5)	C134-H21	Cg...H	0.0141	0.047
DEBA-SWNT(5,5)	H8-C96	Cg...H	0.0141	0.047
DEBA-SWNT(5,5)	C135-H15	Cg...H	0.0091	0.031
DEBA-SWNT(5,5)	C191-C115	Cg…C	0.0096	0.030
DEBA-SWNT(5,5)	C92-C190	Cg…C	0.0139	0.040
DEBA-SWNT(5,5)	C117-C202	Cg…C	0.0198	0.051
DEBA-SWNT(5,5)	C188-C97	Cg…C	0.0144	0.038
DEBA-SWNT(6,6)	O238-C132	Cg...O	0.0175	0.070
DEBA-SWNT(6,6)	C156-H21	Cg...H	0.0131	0.043
DEBA-SWNT(6,6)	C107-H12	Cg...H	0.0125	0.042
DEBA-SWNT(6,6)	H10-C106	Cg...H	0.0147	0.055
DEBA-SWNT(6,6)	H14-C164	Cg...H	0.0069	0.021
DEBA-SWNT(6,6)	C110-H8	Cg...H	0.0134	0.044
DEBA-SWNT(6,6)	C157-H15	Cg...H	0.0091	0.032
DEBA-SWNT(6,6)	O239-C134	Cg…C	0.0125	0.045
DEBA-SWNT(6,6)	C223-C133	Cg…C	0.0093	0.030
DEBA-SWNT(6,6)	C135-C234	Cg…C	0.0186	0.048
DEBA-SWNT(6,6)	C220-C111	Cg…C	0.0142	0.038
DEBA-SWNT(7,7)	O271-C137	Cg...O	0.0162	0.052
DEBA-SWNT(7,7)	C146-O270	Cg...O	0.0187	0.072
DEBA-SWNT(7,7)	C156-H21	Cg...H	0.0122	0.043
DEBA-SWNT(7,7)	H12-C131	Cg...H	0.0103	0.039
DEBA-SWNT(7,7)	H10-C138	Cg...H	0.0111	0.041
DEBA-SWNT(7,7)	C125-H8	Cg...H	0.0140	0.049
DEBA-SWNT(7,7)	C173-H15	Cg...H	0.0089	0.026
DEBA-SWNT(7,7)	C263-C144	Cg…C	0.0094	0.029
DEBA-SWNT(7,7)	C158-C263	Cg…C	0.0089	0.027
DEBA-SWNT(7,7)	C123-C252	Cg…C	0.0105	0.029
DEBA-SWNT(7,7)	C155-C266	Cg…C	0.0162	0.042
DEBA-SWNT(8,8)	C183-O303	Cg...O	0.0127	0.055
DEBA-SWNT(8,8)	C162-O302	Cg...O	0.0168	0.057
DEBA-SWNT(8,8)	H21-C195	Cg...H	0.0110	0.041

DEBA-SWNT(8,8)	C163-H12	Cg...H	0.0117	0.043
DEBA-SWNT(8,8)	H10-C149	Cg...H	0.0078	0.028
DEBA-SWNT(8,8)	H8-C151	Cg...H	0.0126	0.044
DEBA-SWNT(8,8)	H15-C183	Cg...H	0.0085	0.025
DEBA-SWNT(8,8)	C166-C287	Cg…C	0.0102	0.031
DEBA-SWNT(8,8)	C292-C165	Cg…C	0.0132	0.043
DEBA-SWNT(9,9)	C179-O334	Cg...O	0.0163	0.0697
DEBA-SWNT(9,9)	O335-C187	Cg...O	0.0164	0.0539
DEBA-SWNT(9,9)	O334-C143	Cg...O	0.0128	0.0466
DEBA-SWNT(9,9)	H21-C222	Cg...H	0.0128	0.0462
DEBA-SWNT(9,9)	C149-H12	Cg...H	0.0117	0.0392
DEBA-SWNT(9,9)	C148-H10	Cg...H	0.0089	0.0322
DEBA-SWNT(9,9)	H8-C152	Cg...H	0.0139	0.0482
DEBA-SWNT(9,9)	C319-C194	Cg…C	0.0098	0.0295
DEBA-SWNT(9,9)	C193-C327	Cg…C	0.0090	0.0277
DEBA-SWNT(9,9)	C324-C153	Cg…C	0.0098	0.0292
DEBA-SWNT(9,9)	C189-C330	Cg…C	0.0145	0.0391
DEBA-GN	C172-H24	Cg...H	0.0029	0.0086
DEBA-GN	C212-H20	Cg...H	0.0119	0.0389
DEBA-GN	C218-H21	Cg...H	0.0090	0.0356
DEBA-GN	C192-O289	Cg...O	0.5540	0.0216

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