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Exploring adsorption of neutral aromatic pollutants onto graphene nanomaterials via molecular dynamics simulations and theoretical linear solvation energy relationships

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Table S1. 35 compounds in the training set and 8 compounds in the validation set

Group	Compound	Substituents	Group	Compound	Substituents
V	benzene (PhH)		V	p-xylene (PXYL)	$-CH_3$
T	chlorobenzene (PhCl)	-Cl	T	4-chlorotoluene (PCLT)	$-CH_3$, -Cl
T	bromobenzene (PhBr)	-Br	T	4-nitrotoluene (NoT)	$-NO_2$, $-CH_3$
T	iodobenzene (PhI)	-I	T	(3-methylphenyl) methanol (MeBl)	$-CH_3$, $-CH_2OH$
T	phenol (PhOH)	-OH	V	4-chloroanisole (ClAn)	-Cl, $-OCH_3$
T	benzonitrile (PhCN)	-CN	T	4-chloroacetophenone (ClAh)	-Cl, $-C(O)CH_3$
T	nitrobenzene (PhNO2)	$-NO_2$	T	1,3-dinitrobenzene (DNIN)	$-NO_2$
T	toluene (PhMe)	$-CH_3$	V	methyl 2-methyl benzoate (MMBa)	$-CH_3$, $-C(O)OCH_3$
T	phenylmethanol (PhMl)	$-CH_2OH$	T	4-chloroaniline (PhAm)	-Cl, $-NH_2$
V	ethylbenzene (PhEt)	$-CH_2CH_3$	T	3,5-dimethylphenol (dMPl)	-OH, $-CH_3$
T	propylbenzene (PhPr)	$-CH_2CH_2CH_3$	T	hexabromobenzene (HBB)	-Br
V	acetophenone (BzMe)	$-C(O)CH_3$	T	pentabromotoluene (PBT)	-Br, $-CH_3$
T	methylbenzoate (BzOMe)	$-C(O)OCH_3$	T	1,2-dibromo-4-(1,2-dibromoethyl)-cyclohexane (TBE)	-Br, $-CHBrCH_2Br$
T	2-phenylethanol (PhEl)	$-CH_2CH_2OH$	T	tetrabromo-*o*-chlorotoluene (TBCT)	-Cl, -Br, $-CH_3$
T	phenylacetate (PhOAc)	$-OC(O)CH_3$	T	naphthalene (NAFT)	
T	ethylbenzoate (BzOEt)	$-C(O)OCH_2CH_3$	T	biphenyl (PhPh)	
T	4-fluorophenol (FPl)	-OH, -F	T	1-methylnaphthalene (MeNh)	$-CH_3$
T	3-chlorophenol (ClPl)	-OH, -Cl	T	BDE209 (B209)	-O-, -Br
V	3-bromophenol (BrPl)	-OH, -Br	T	BDE47 (B47)	-O-, -Br
T	m-cresol (mCr)	-OH, $-CH_3$	T	BDE99 (B99)	-O-, -Br
V	p-cresol (PCRO)	$-CH_3$, -OH	T	BDE207 (B207)	-O-, -Br
T	4-ethylphenol (EPHE)	-OH, $-CH_2CH_3$			

T and V represent training set and validation set, respectively.

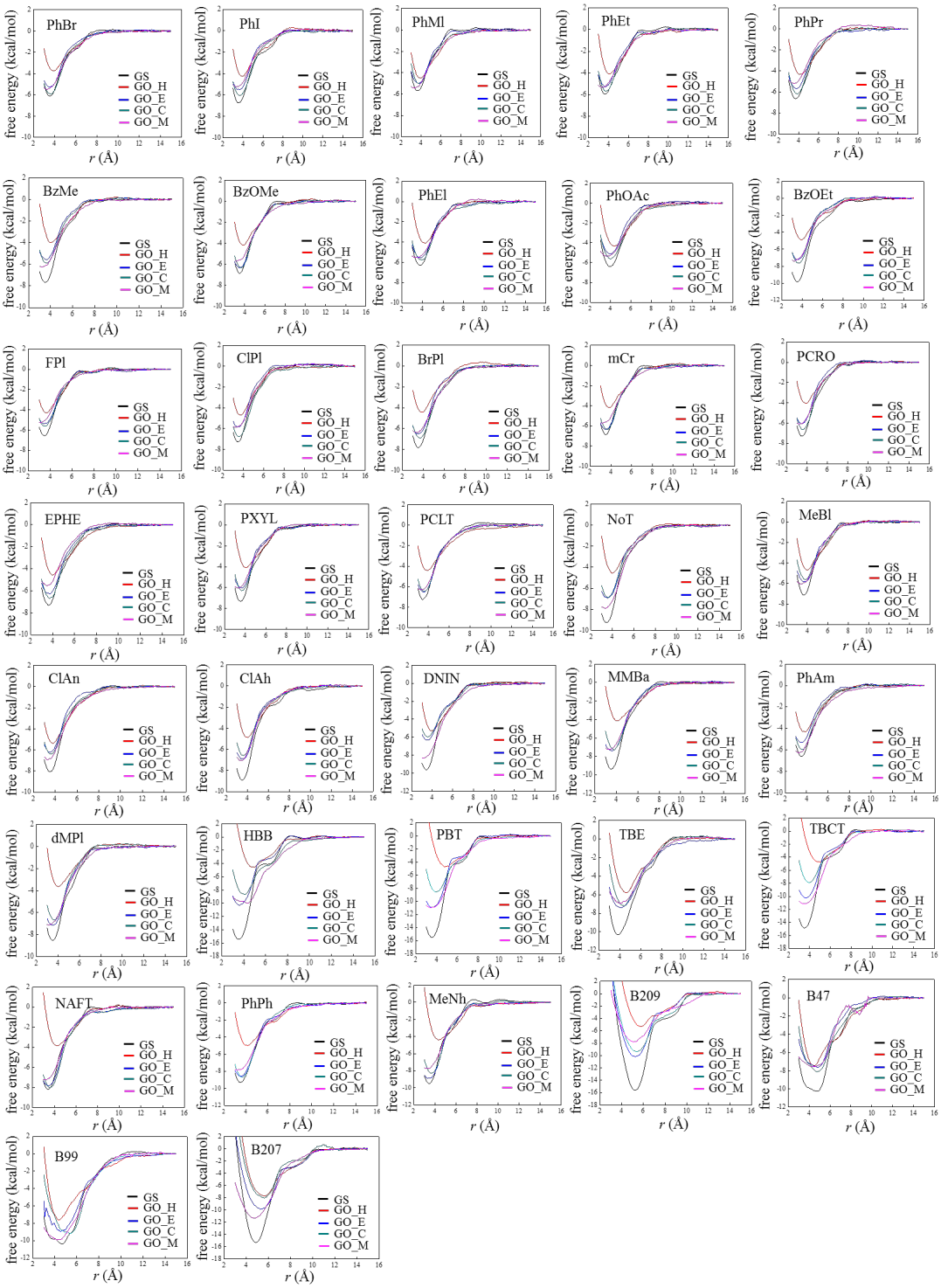

Fig. S1 Calculated free energy versus distance (*r*) between the center-of-mass for 37 organic compounds and the surface of graphene or graphene oxide nanosheets.

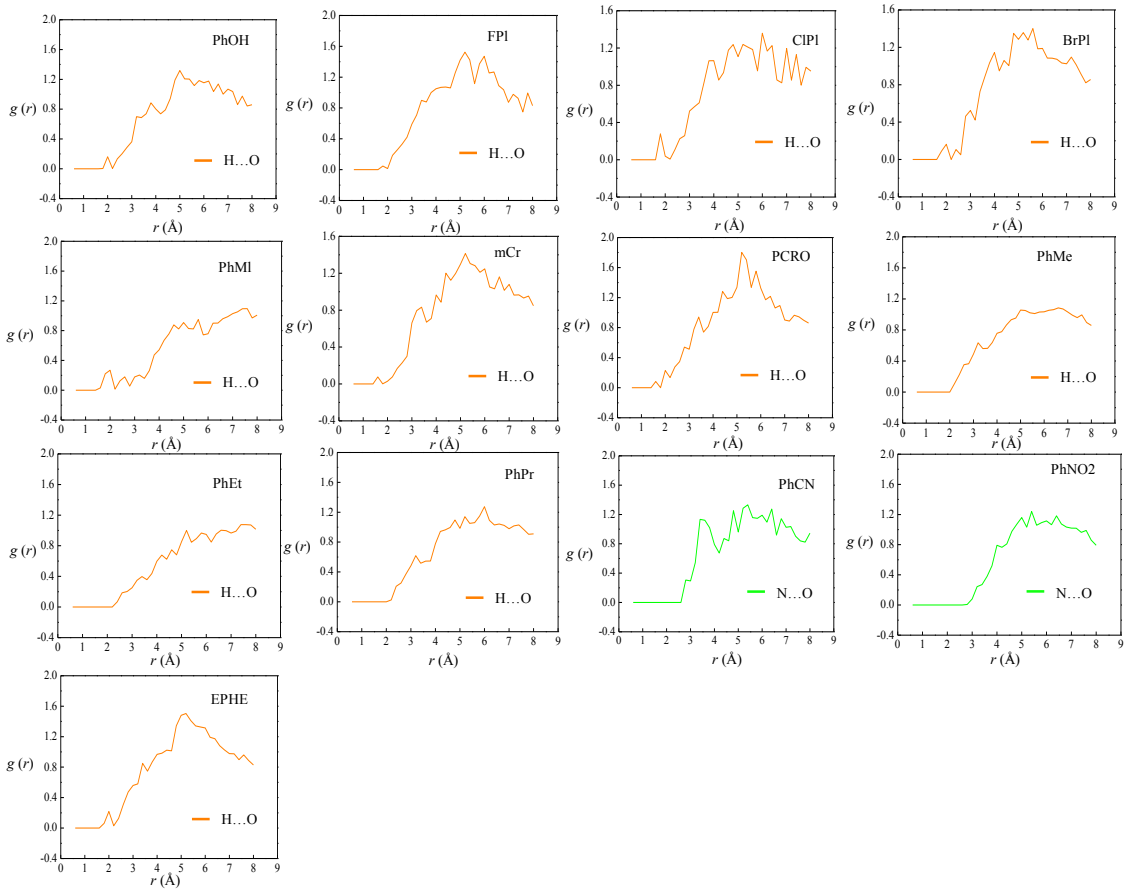

Fig. S2 Radial distribution functions (RDFs) on GO_E. H…O: RDFs for H atom in the substituent of a compound relative to the O atom on GO_E; N…O: RDFs for N atom in the substituent of a compound relative to the O atom on GO_E.

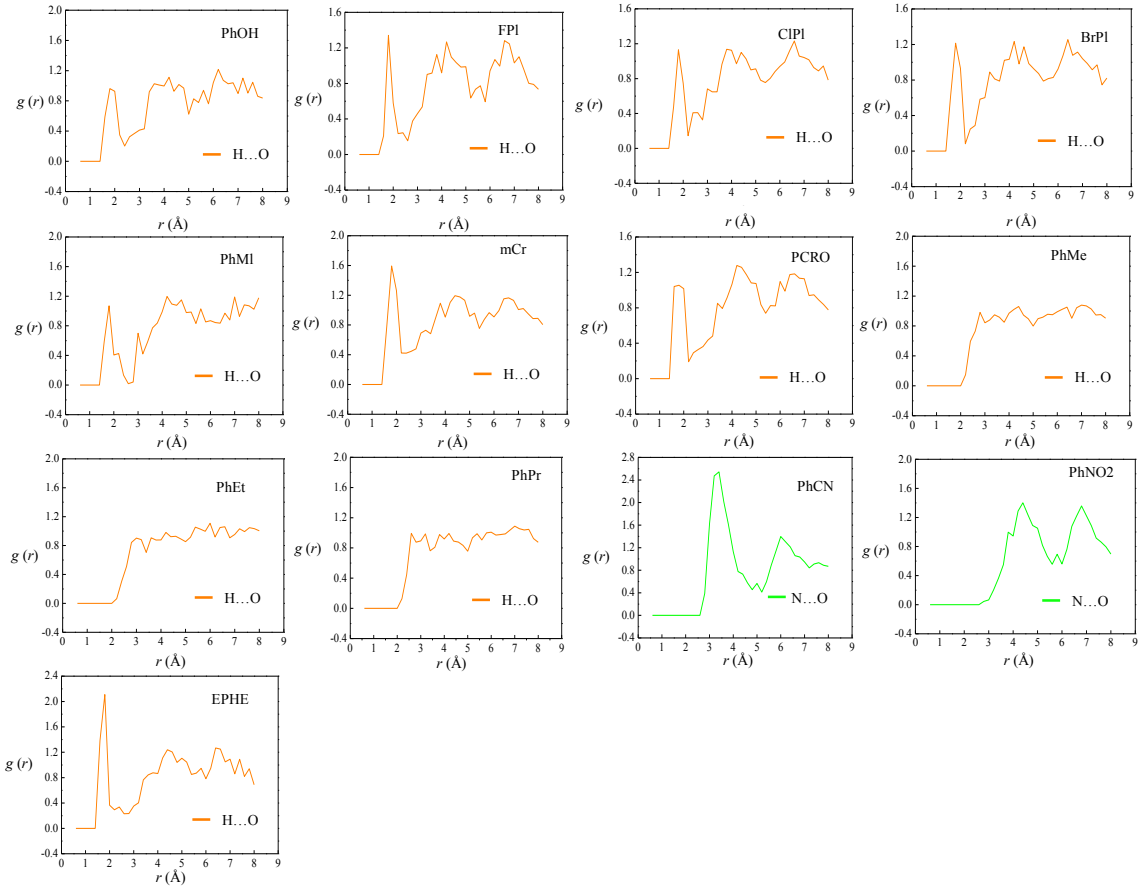

Fig. S3 RDFs on GO_C. H…O: RDFs for H atom in the substituent of a compound relative to the O atom on GO_C; N…O: RDFs for N atom in the substituent of a compound relative to the O atom on GO_C.

SI1. Details for computing the electrostatic potential distribution with density functional theory (DFT) method

In the density functional theory (DFT) computation, the graphene is a 8 × 8 × 1 supercell, which consists of 128 carbon atoms, while the graphene oxide with the hydroxyl and epoxy groups, includes 128 carbon, 24 hydrogen and 36 oxygen atoms. For graphene oxide, its O/C ratio is 0.28125, consistent with GO_M.

DMol^3 program[1,2] was applied for carrying out the DFT computations. Before computing the electrostatic potential distribution for the graphene and graphene oxide, we optimized their structures with Perdew-Burke-Ernzerhof generalized gradient approximation (GGA-PBE)[3] and double-numerical basis with polarization functions (DNP).[4,5] Besides, the PBE+D2[6] method has also been used. The Gamma point was utilized for sampling in Brillouin-zone, and a Methfessel-Paxton smearing of 0.005 Ha was used for doing Brillouin-zone integration.

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