Supporting Information
for the article

Fast and Accurate Computational Modeling of Adsorption on Graphene: A Dispersion Interaction Challenge

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Table S1. Calculated adsorption energy (E_{ads}, in kcal/mol) and calculated distance (*l*, in Å) for adsorption of various molecules on the $C_{54}H_{18}$ part of graphene sheet with different GNORM parameter.[a]

Entry	Molecule	Dispersion corrected at PM6-DH2 level		Without correction at PM6 level	
		GNORM=0.5	GNORM=0.01	GNORM=0.5	GNORM=0.01
1	CO_2	-3.8 (3.30)	-3.9 (3.25)	-0.8 (3.50)	-0.8 (3.45)
2	CO	-2.7 (3.14)	-2.7 (3.11)	-0.8 (3.15)	-0.8 (3.15)
3	NH_3 [r]	-4.8 (3.19)	-4.8 (3.19)	-2.0 (3.24)	-2.0 (3.23)
4	CH_4	-3.1 (3.28)	-3.1 (3.28)	-0.4 (3.38)	-0.4 (3.55)
5	H_2	-1.0 (3.07)	-1.0 (3.04)	-0.01 (3.13)	-0.1 (3.03)
6	H_2O	-4.2 (3.19)	-4.2 (3.18)	-2.2 (3.21)	-2.2 (3.20)
7	N_2	-2.9 (3.24)	-2.9 (3.24)	-0.6 (3.40)	-0.6 (3.40)
8	Benzene	-11.1 (3.29)	-11.1 (3.29)	-1.0 (3.50)	-1.0 (3.49)
9	Naphthalene	-17.5 (3.31)	-17.5 (3.32)	-1.5 (3.50)	-1.6 (3.51)
10	Cyclohexane	-8.3 (3.78)	-9.0 (3.69)	-1.1 (4.00)	-1.3 (3.89)
11	Coronene	-34.8 (3.22)	-35.3 (3.39)	-2.5 (3.53)	-2.6 (3.56)
12	Ovalene	-42.9 (3.34)	-42.9 (3.38)	-2.7 (3.53)	-3.1 (3.56)
13	$C_{54}H_{18}$	-58.6 (3.40)	-58.7 (3.37)	-4.5 (3.58)	-4.5 (3.58)

[a] The values of adsorption energy are given without parenthesis and calculated distance in parenthesis (see also Table 1).

The variation of gradient norm from 0.5 to 0.01 by GNORM keyword led to insignificant influence on the values of adsorption energy (Table S1) with the exception of cyclohexane (the difference of 0.7 kcal/mol at the PM6-DH2 level) and coronene (the difference of 0.5 kcal/mol). The influence of the gradient norm variation was more pronounced for the calculated distances between the bound molecule and C_{54} plane (Table S1). It should be noted, that in some cases decreasing GNORM parameter from 0.5 to 0.01 markedly increased the calculation time.

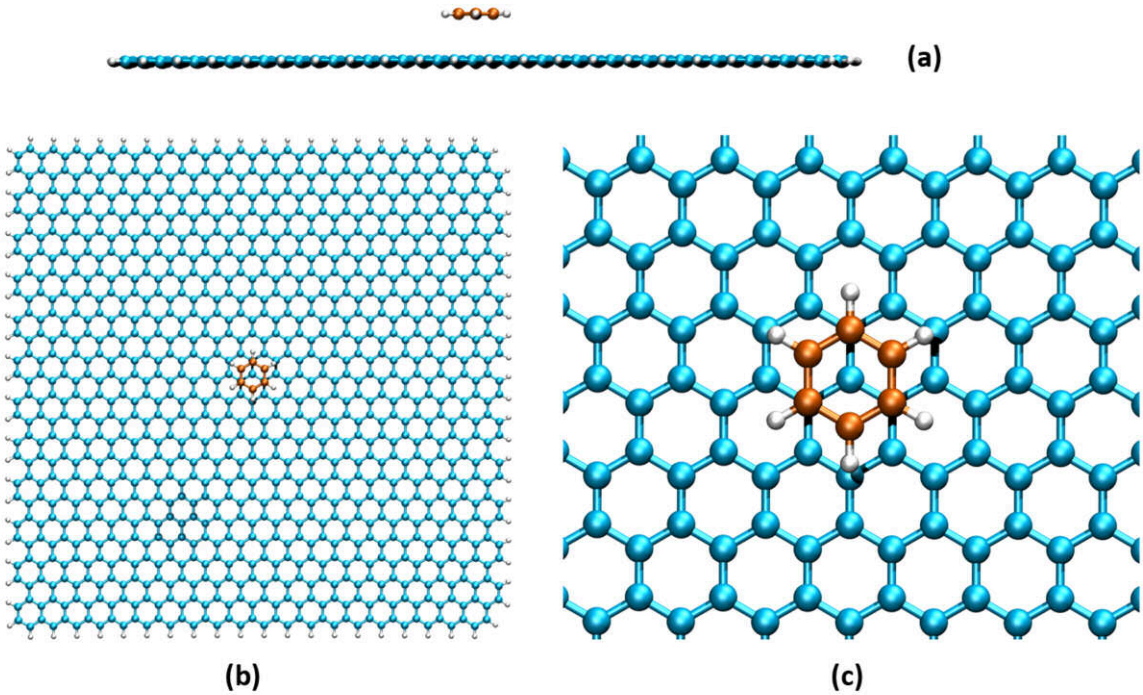

Figure S1. Optimized molecular structure of intermolecular complex of benzene with $C_{1006}H_{88}$ sheet: (a) – side view, (b) – top view, (c) – scaled-up top view of adsorption core. The carbon atoms of benzene molecule and $C_{1006}H_{88}$ sheet are depicted by different colors for clarity.

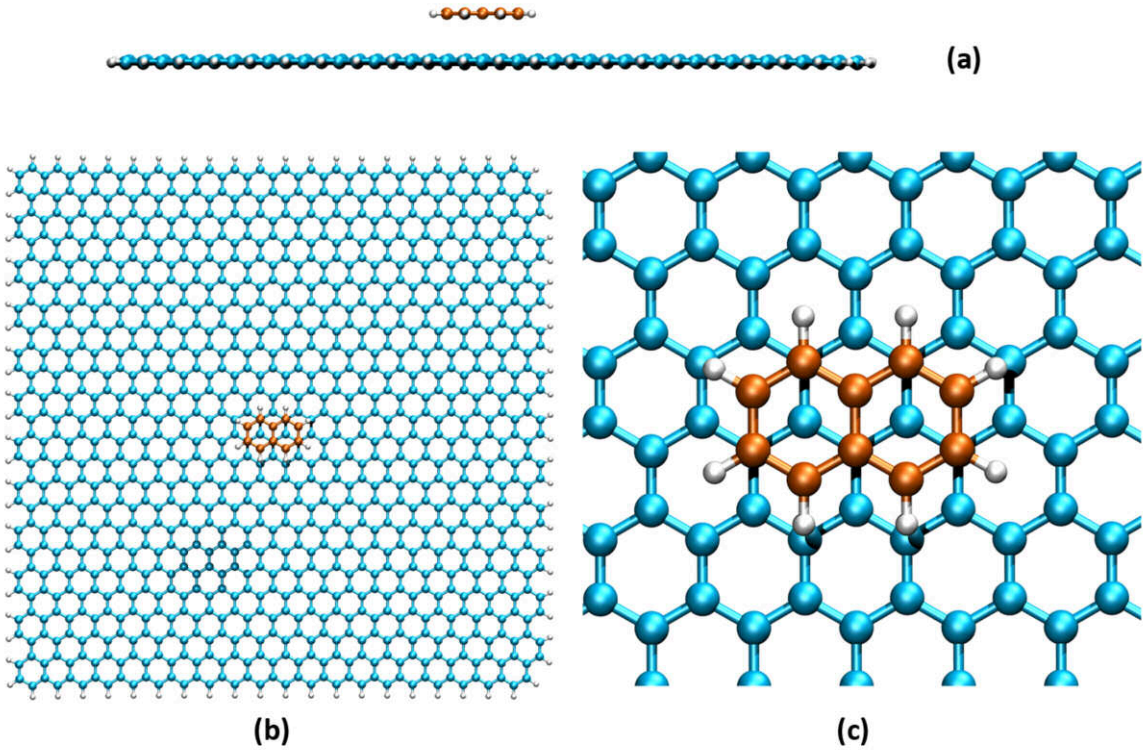

Figure S2. Optimized molecular structure of intermolecular complex of naphthalene with $C_{1006}H_{88}$ sheet: (a) – side view, (b) – top view, (c) – scaled-up top view of adsorption core.

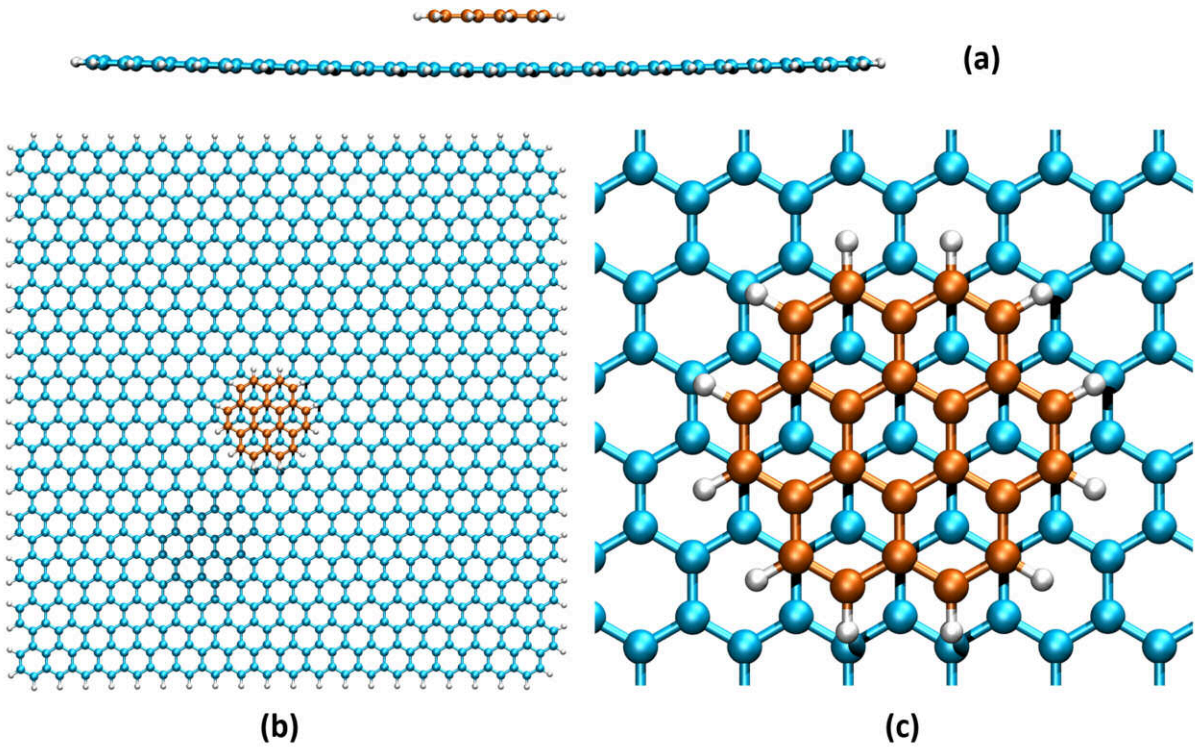

Figure S3. Optimized molecular structure of intermolecular complex of coronene with $C_{1006}H_{88}$ sheet: (a) – side view, (b) – top view, (c) – scaled-up top view of adsorption core.

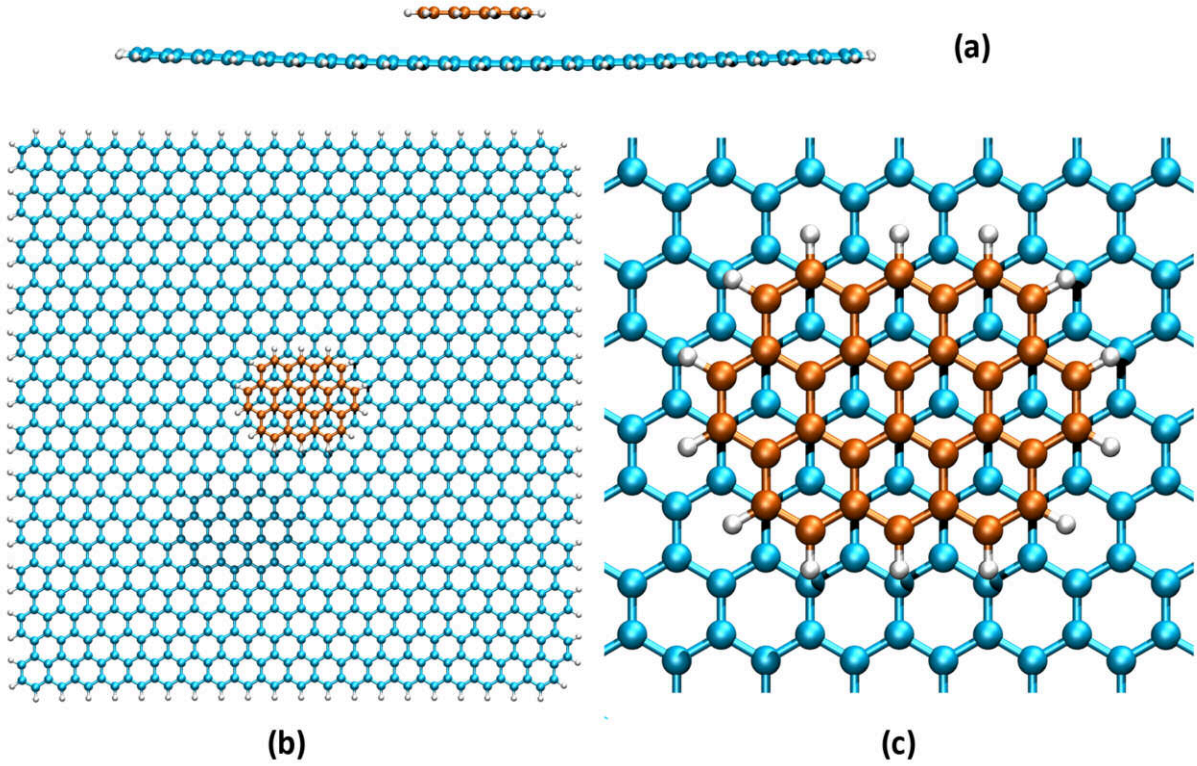

Figure S4. Optimized molecular structure of intermolecular complex of ovalene with $C_{1006}H_{88}$ sheet: (a) – side view, (b) – top view, (c) – scaled-up top view of adsorption core.

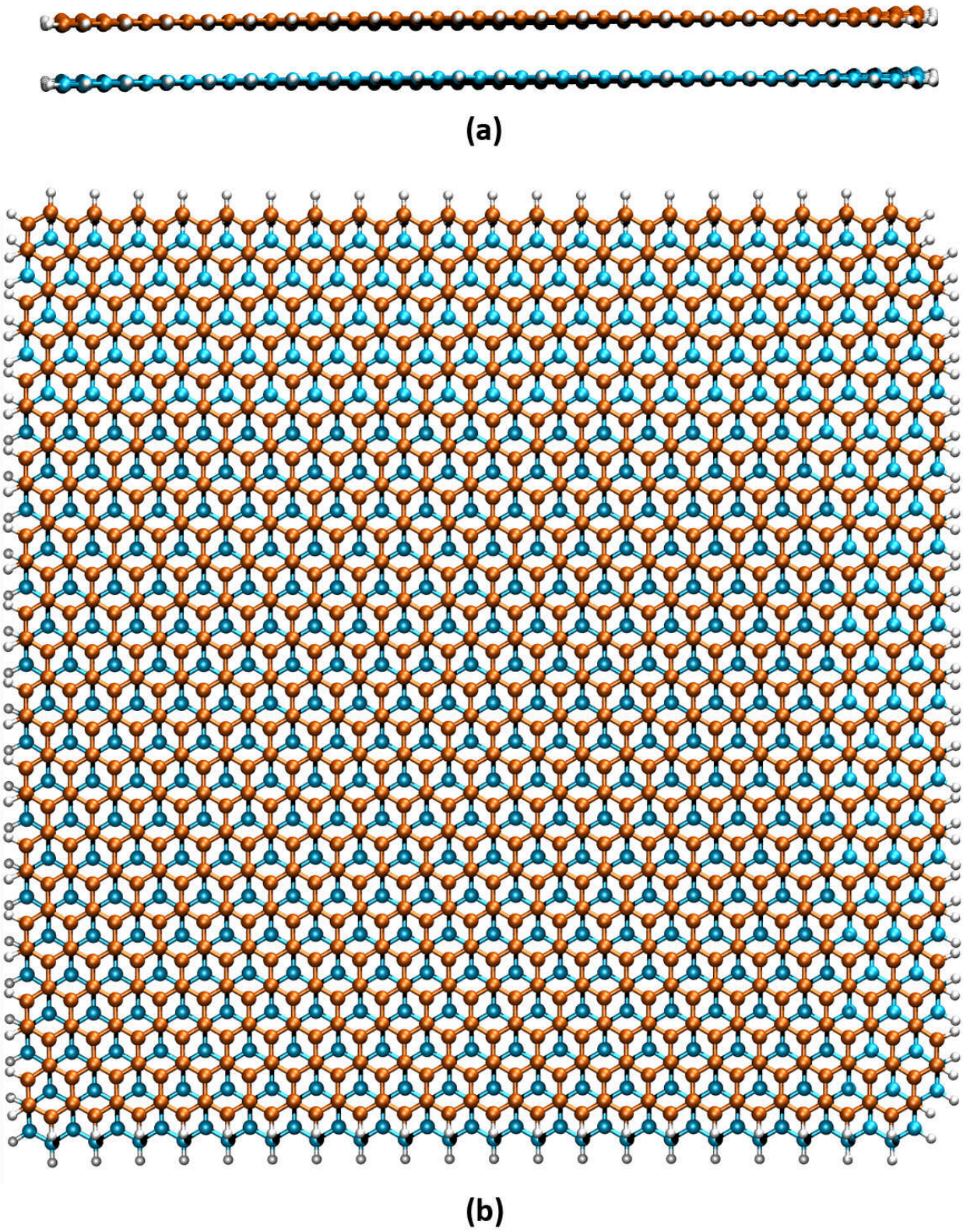

Figure S5. Optimized molecular structure of intermolecular complex of the two $C_{1006}H_{88}$ sheets: (a) – side view, (b) – top view.