Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supplementary Information for

Potential models for the simulation of methane adsorption on graphene: development and CCSD(T) benchmarks

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Table S1. Benzene-methane and naphthalene-methane interaction energies, D_e, and equilibrium distances, R_e.

Benzene-methane				
	B97D		CCSD(T)	
Conformation	D_e (kcal/mol)	R_e (Å)	D_e (kcal/mol)	R_e (Å)
H-up	1.17	3.71	1.23[a]	3.6[a]
2H-up	1.28	3.67	1.32[a]	3.6[a]
3H-up	1.44	3.66	1.45[a]	3.8[a]
Naphthalene-methane				
	B97D		CCSD(T)	
Conformation	D_e (kcal/mol)	R_e (Å)	D_e (kcal/mol)	R_e (Å)
H-up	1.96	3.40	1.94[b], 2.126[c]	—
2H-up	1.88	3.54	1.78[b], 1.86[a], 2.088[c]	3.6[a]
3H-up	1.66	3.72	1.40[b]	—

(a) S. Tsuzuki, K. Honda, T. Uchimaru, M. Mikami and K. Tanabe, *J. Am. Chem. Soc.*, 2000, **122**, 3746–3753

(b) Calculated at the DFT equilibrium distance.

(c) D.G. Smithand, K. Patkowski, *J. Chem. Theory Comput.*, 2013, **9**, 370–389.

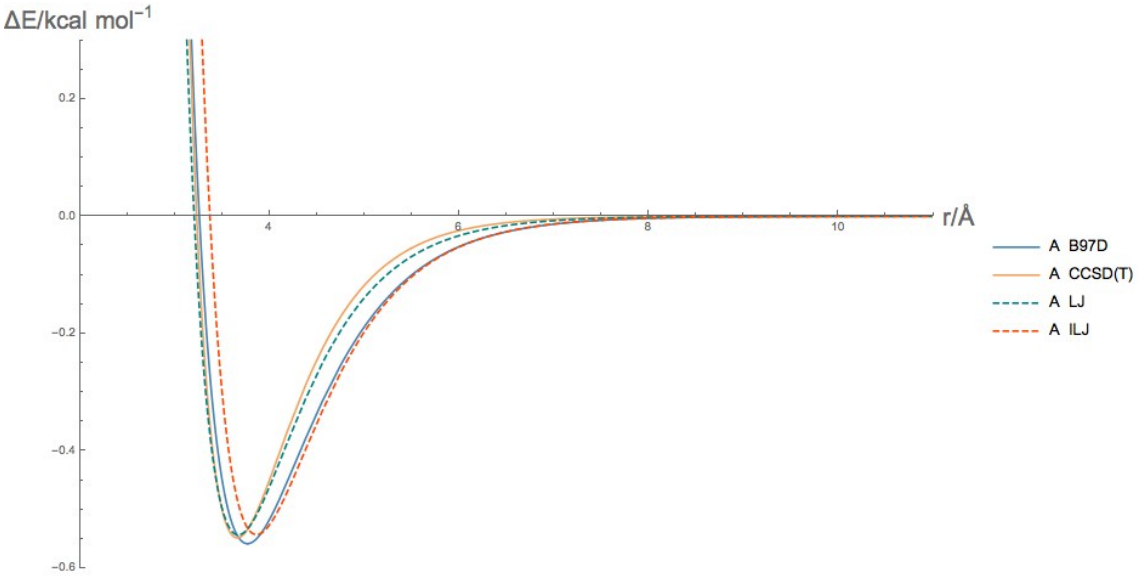

Figure S1. Potential energy profile for the intermolecular interaction in methane dimer in A (face-face) conformation.

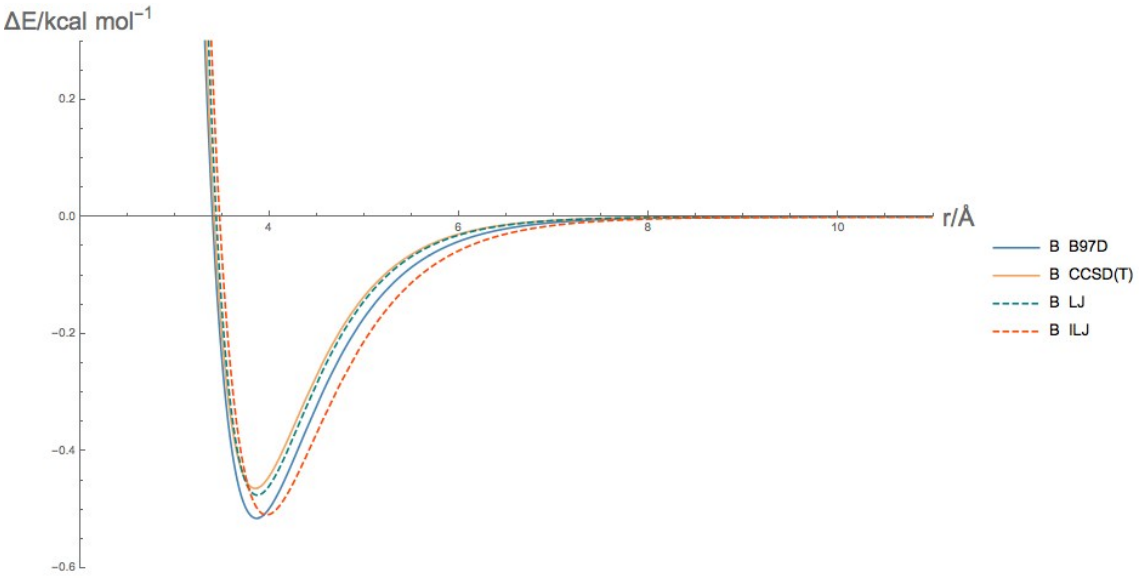

Figure S2. Potential energy profile for the intermolecular interaction in methane dimer in B (face-edge) conformation.

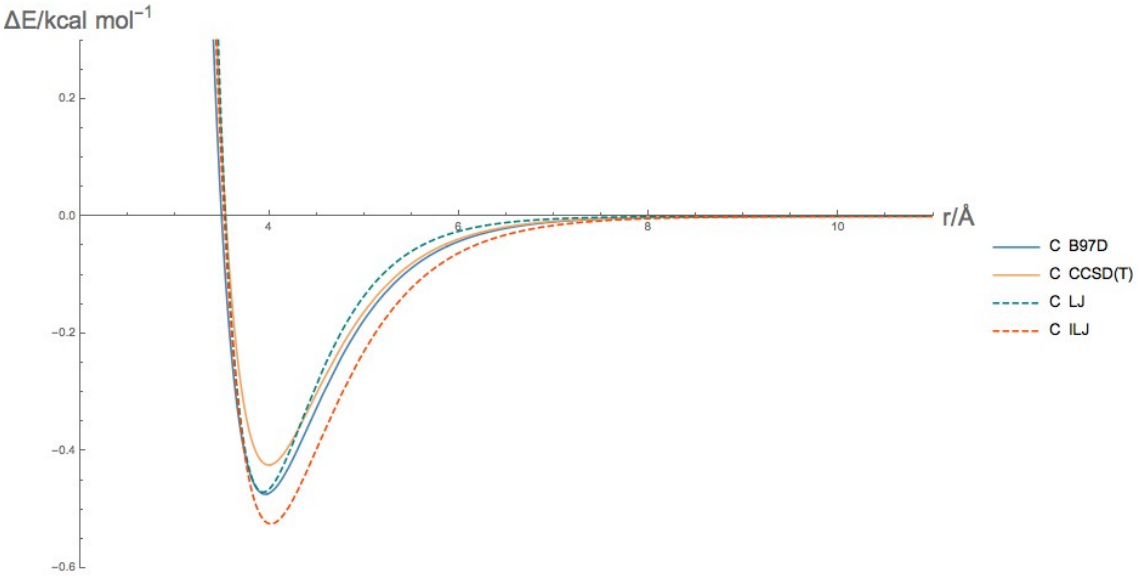

Figure S3. Potential energy profile for the intermolecular interaction in methane dimer in C (edge-edge) conformation.

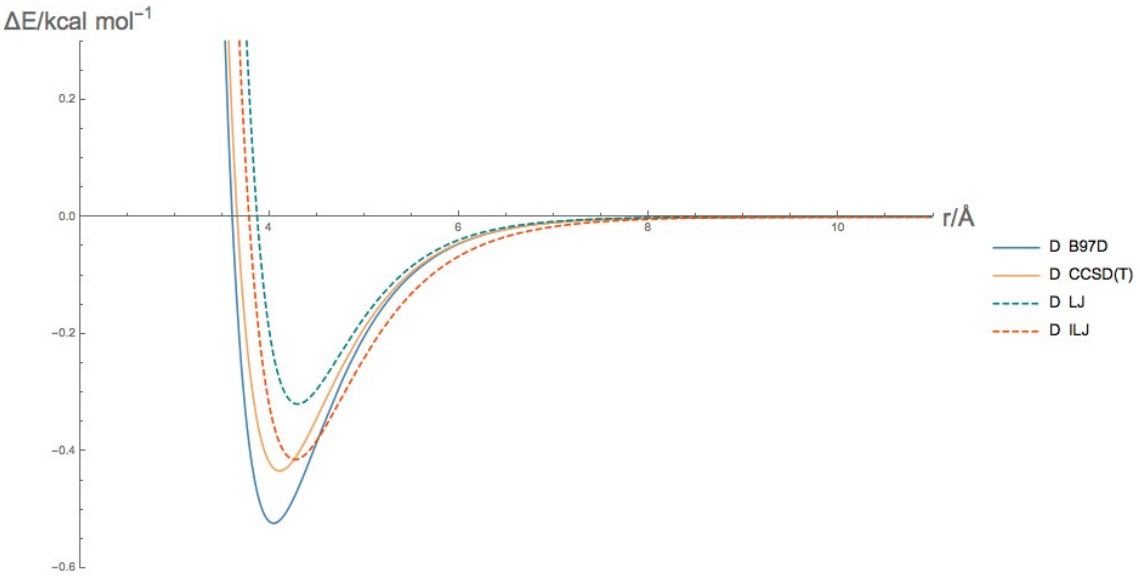

Figure S4. Potential energy profile for the intermolecular interaction in methane dimer in D (face-vertex) conformation.

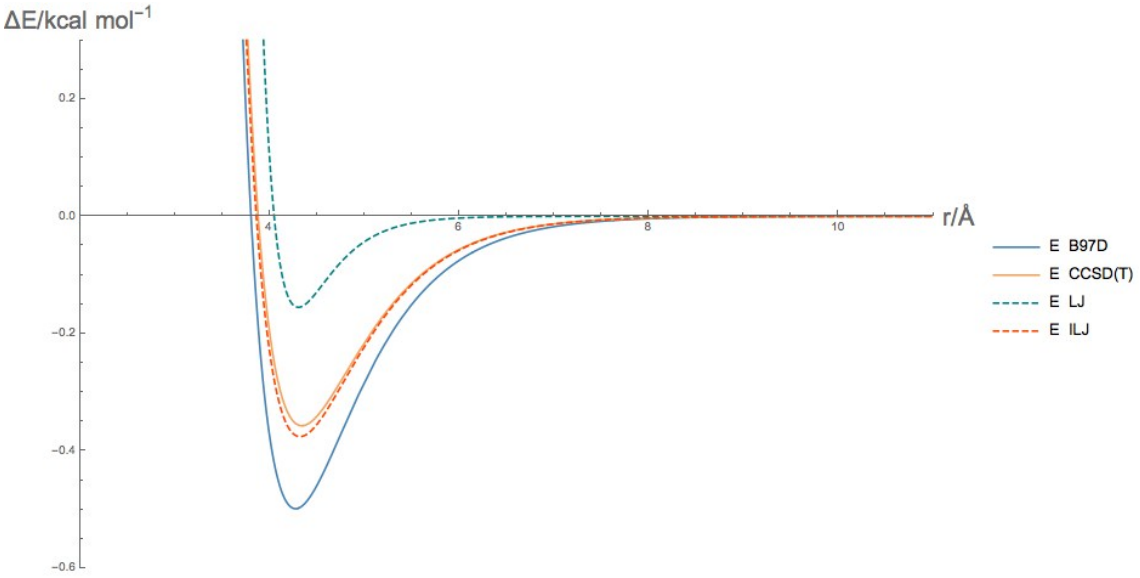

Figure S5. Potential energy profile for the intermolecular interaction in methane dimer in E (edge-vertex) conformation.

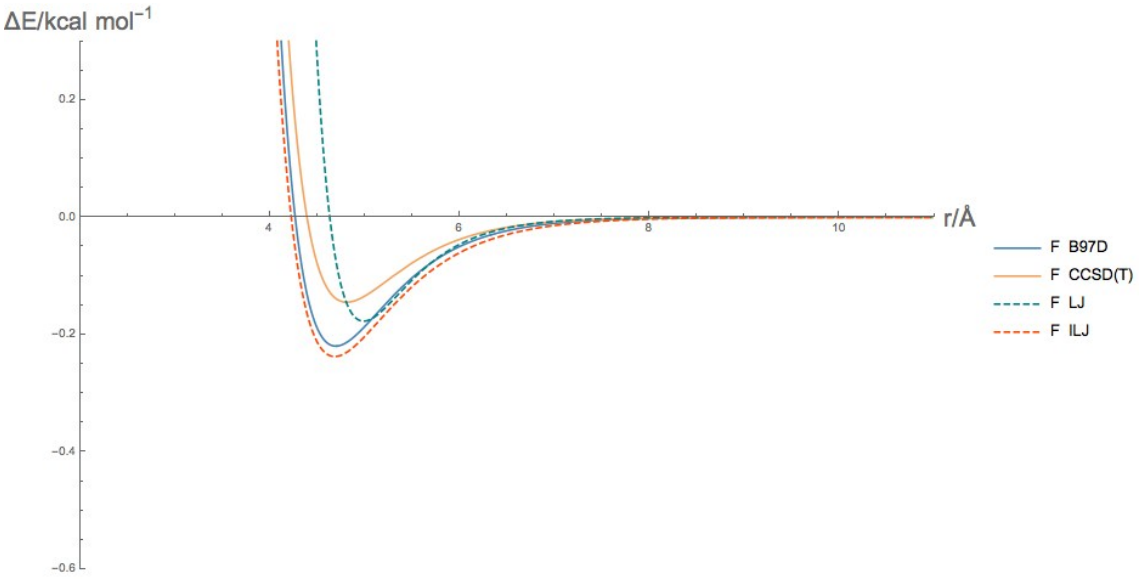

Figure S6. Potential energy profile for the intermolecular interaction in methane dimer in A (vertex-vertex) conformation.