Supplementary Materials: Polycyclic Aromatic Hydrocarbons Adsorption onto Graphene: A DFT and AIMD Study

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Table S1. Calculated adsorption energies of polycyclic aromatic hydrocarbons (PAHs) adsorption onto Gr for different initial configurations (refer to the initial configurations (1)–(6) illustrated in Figure 1) by Perdew–Burke–Ernzerhof (PBE)-D3 (E_{ad}; in eV).

PAHs	E_{ad}					
	Hollow (1)	**Top (2)**	**Top (3)**	**Bridge (4)**	**Bridge (5)**	**Bridge (6)**
Nap	−0.598	**−0.638**	**−0.638**	−0.635	−0.632	−0.632
Ace	−0.714	**−0.762**	**−0.762**	−0.743	−0.757	−0.757
Acp	−0.696	−0.728	**−0.731**	−0.713	−0.730	−0.730
Flu	−0.779	−0.802	−0.801	−0.802	**−0.812**	−0.801
Phe	−0.813	−0.866	**−0.870**	−0.866	−0.862	−0.862
Ant	−0.819	**−0.872**	**−0.872**	−0.868	−0.867	−0.862
Flt	−0.916	−0.932	−0.954	−0.932	**−0.955**	**−0.955**
Pyr	−0.897	−0.950	−0.960	**−0.961**	−0.948	−0.950
BaA	−1.030	**−1.101**	−1.092	−1.093	−1.098	−1.092
Chr	−1.025	**−1.099**	−1.086	−1.092	−1.086	−1.091
BbF	−1.128	−1.158	−1.178	−1.158	−1.178	**−1.182**
BkF	−1.135	**−1.187**	−1.170	−1.166	−1.182	−1.174
BaP	−1.114	−1.189	−1.189	**−1.190**	−1.178	−1.177
InP	−1.222	**−1.269**	−1.262	−1.259	−1.254	−1.265
DbA	−1.236	−1.323	−1.323	−1.313	**−1.324**	−1.309
BeP	−1.190	**−1.281**	**−1.281**	−1.267	−1.274	−1.273