Supplementary Information

for

Understanding the Thermodynamics of the Binding of PAMAM Dendrimers to Graphene: a Combined Analytical and Simulation Study

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1. Chemical Structure of the Dendrimer

Shown in figure S1 are the details of the various amines of a G1 PAMAM dendrimer. At neutral pH (~ 7) the primary amines (circled in green) will be protonated. At low pH (~ 4) the tertiary amines at the core and the branch points (circled in blue) will also be protonated.
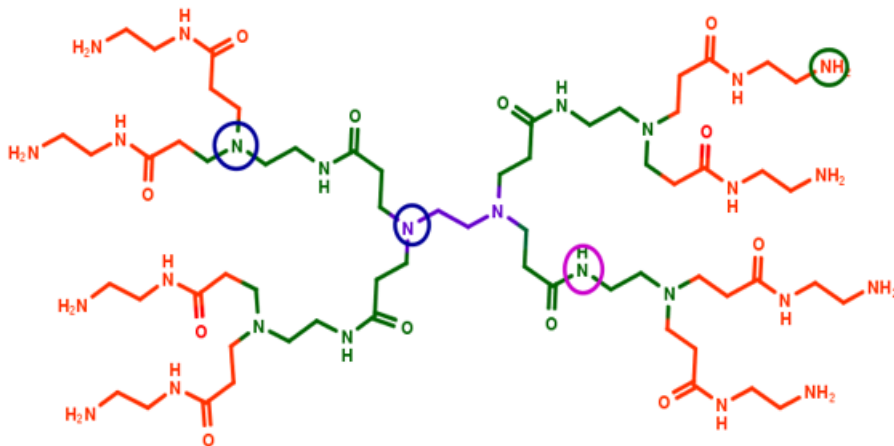

Figure S1: Schematic of G1 PAMAM dendrimer. The primary, secondary and tertiary amines are circled in green, pink and blue respectively.

2. Equilibrium Simulation Details

Table S1: Details of the Equilibrium simulations and some of the structural parameters of the dendrimer. *Bulk* stands for the bulk simulation and *Ads* stands for the simulations with graphene sheet.

Case	Simulation time (ns)		$\langle R_g \rangle$ (Å)		$\langle R_g \rangle_{\parallel}$ (Å) (Ads)	$\langle R_g \rangle_{\perp}$ (Å) (Ads)	Height (Å) (Ads)
	Bulk	Ads	Bulk	Ads			
G3NP	70	55	12.5	13.8	12.1	6.5	29.3
G3P	90	100	15.3	17.3	15.9	7.0	31.8
G3AC	70	80	19.6	19.4	17.7	8.1	33.2
G4NP	70	120	16.1	17.4	15.9	7.1	29.9
G4P	90	85	20.5	22.1	19.0	11.4	45.4
G4AC	70	80	24.4	24.5	20.7	13.1	52.3

3. Comparing the PMF profiles from WHAM and force integration methods

The total PMF profiles from force integration are obtained by summing the contributions from dendrimer-graphene, dendrimer-water and dendrimer-ion interactions presented in figure 7 of main-text.
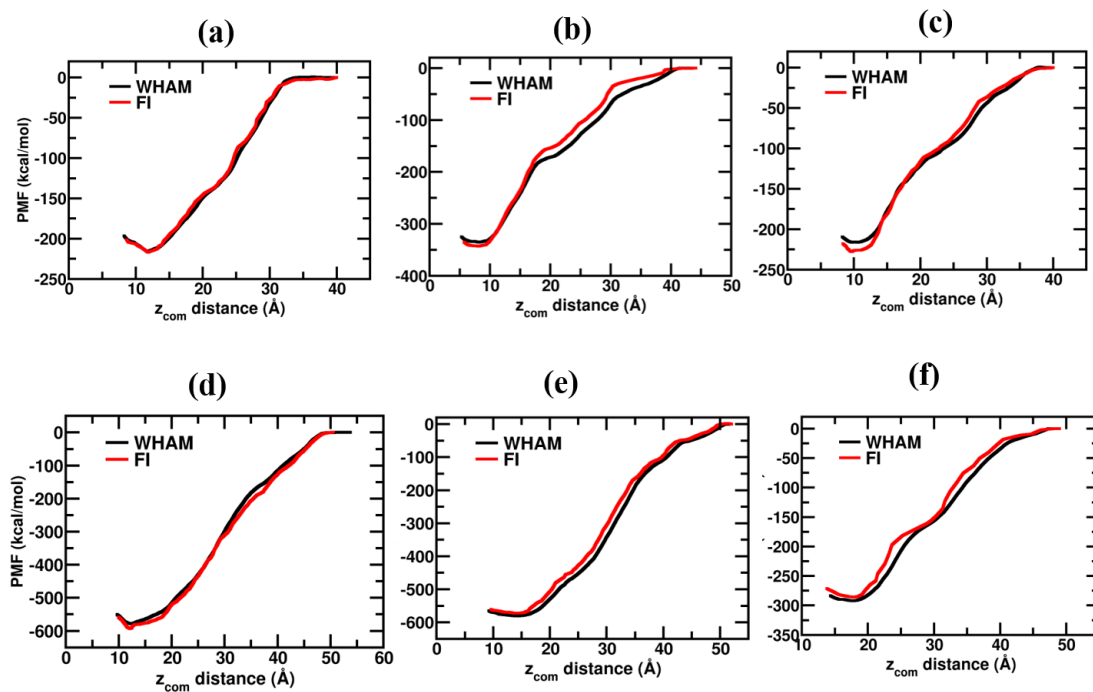

Figure S2: Comparing the PMF profiles from WHAM and force integration (FI) for (a) G3NP (b) G3P (c) G3AC (d) G4NP (e) G4P and (f) G4AC.