Supplementary Information

for

pH and Generation Dependent Morphologies of PAMAM Dendrimers on Graphene Substrate

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Protonation level of the dendrimer is a function of the pH level of the medium. The protonation sites at various pH levels are shown in figure S1. While mapping the adsorbed dendrimer structures to various morphologies observed in our study, we calculate the orientation of the vector joining the core of the dendrimer to each of the terminal amines. A schematic of one such vector is also shown in figure S1.
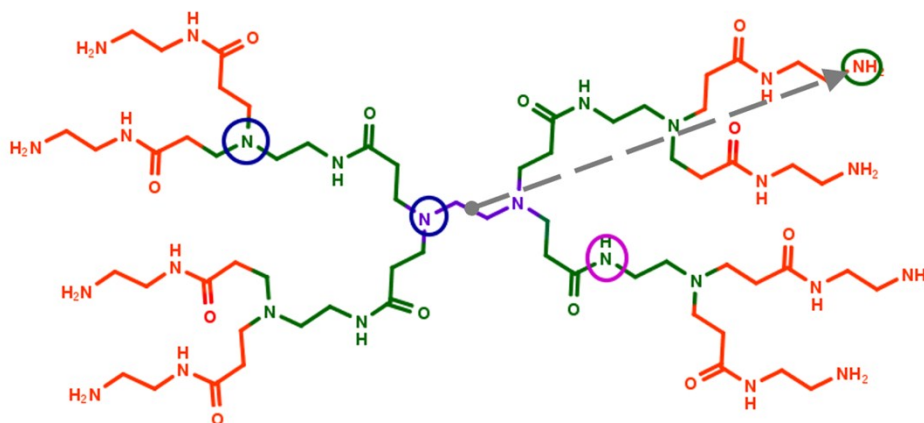

Figure S1: Schematic of G1 PAMAM dendrimer at high pH. Primary amines are circled in green. Secondary amines are colored in pink and the teritary amines in blue. At high pH (pH ~ 10), no amines get protonated. At neutral pH (pH ~ 7) levels, the primary amines on the terminals get protonated. At low pH (pH ~ 4) values even the tertiary amines at the branch points, core get protonated.
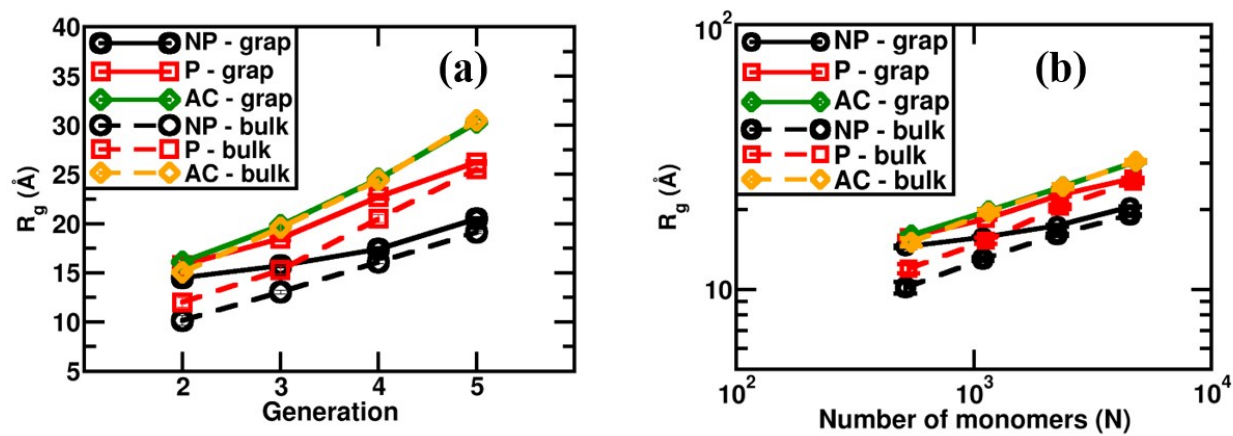
Figure S2: R_g as a function of generation for (a) grap and bulk cases at NP, P and AC. (b) A log-log plot of R_g as a function of number of monomers for grap and bulk cases at NP (circles), P (squares) and AC (diamonds).

Orientation of the vector joining core of the dendrimer to the terminal amine (figure S1) with respect to the sheet normal is an important parameter to systematically quantify the adsorbed dendrimer morphologies. In figure S3 the average orientations are plotted for G2 and G3 dendrimers at all pH and salt levels considered. Similarly figure S4 illustrates the orientations for G4 and G5 dendrimers.
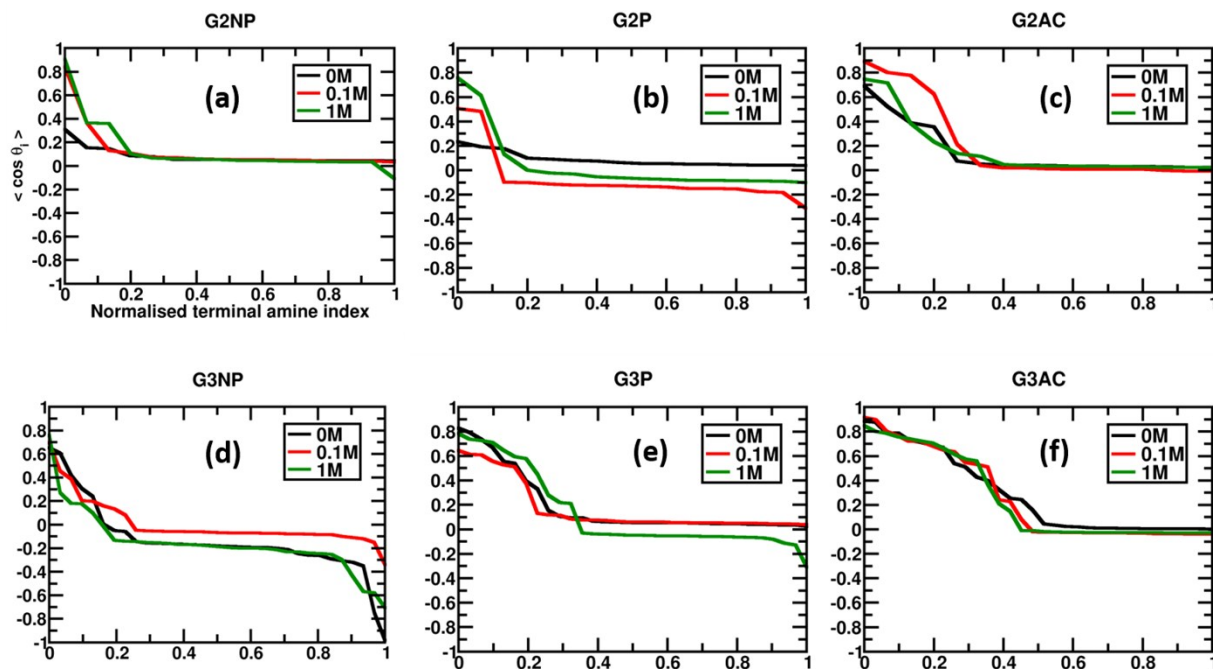

Figure S3: Average orientation of vector joining the terminal amines and the center of mass of the dendrimer at all the three salt levels considered for (a) G2NP (b) G2P (c) G2AC (d) G3NP (e) G3P and (f) G3AC dendrimers.
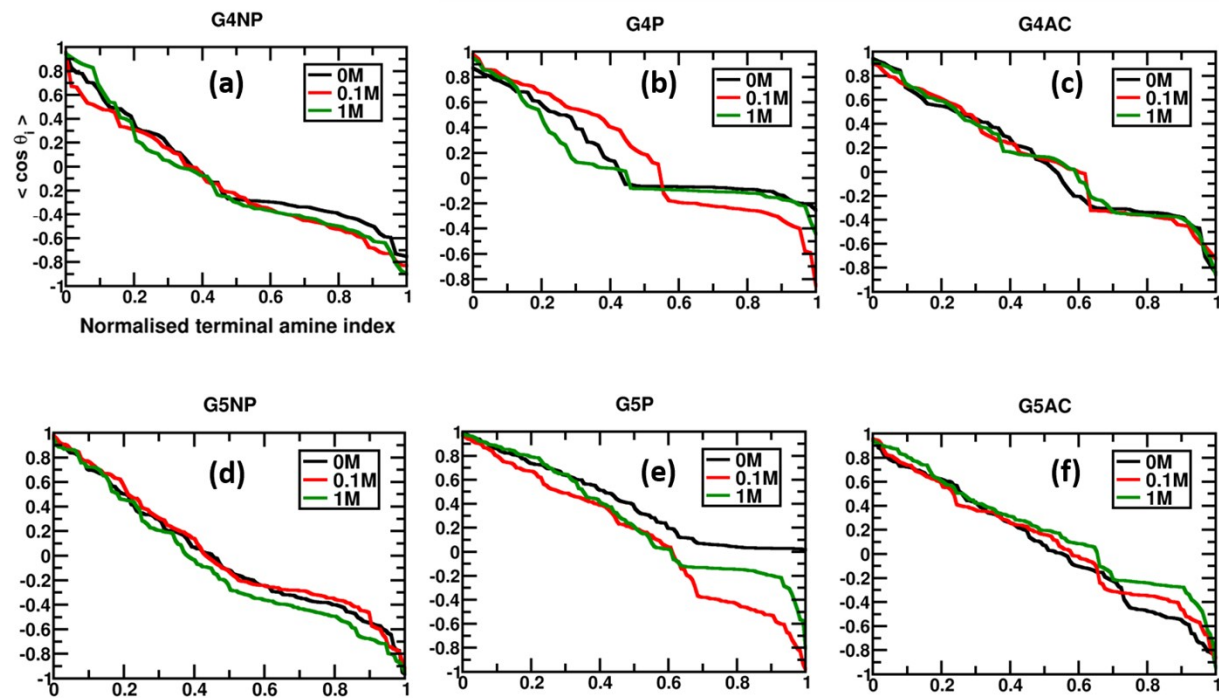
Figure S4: Same as figure S3 but for G4 and G5 dendrimers.