

Supplementary Materials

Structure of Carbon Nanotube-dendrimer composite

V.Vasumathi, Debabrata Pramanik, A. K. Sood and Prabal K Maiti

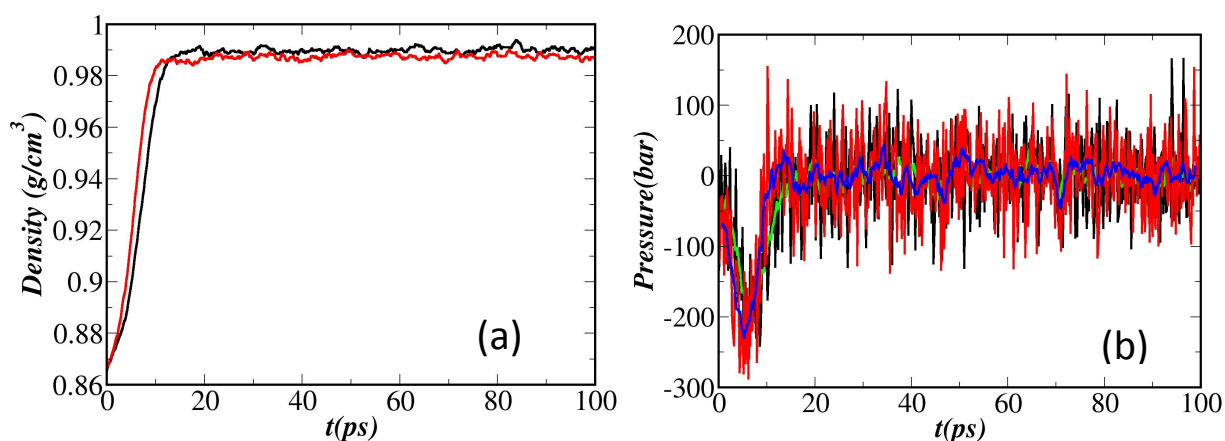


Figure S1: Equilibration of (a) density and (b) pressure as a function of time at the beginning of the simulation in the case of protonated and non-protonated PAMAM dendrimer of generation 3. Red and black lines represent the non-protonated and protonated cases respectively. Green and blue colors in (b) represent the running average of the pressure in both the cases. Subsequently the simulation was continued at the same density and pressure.

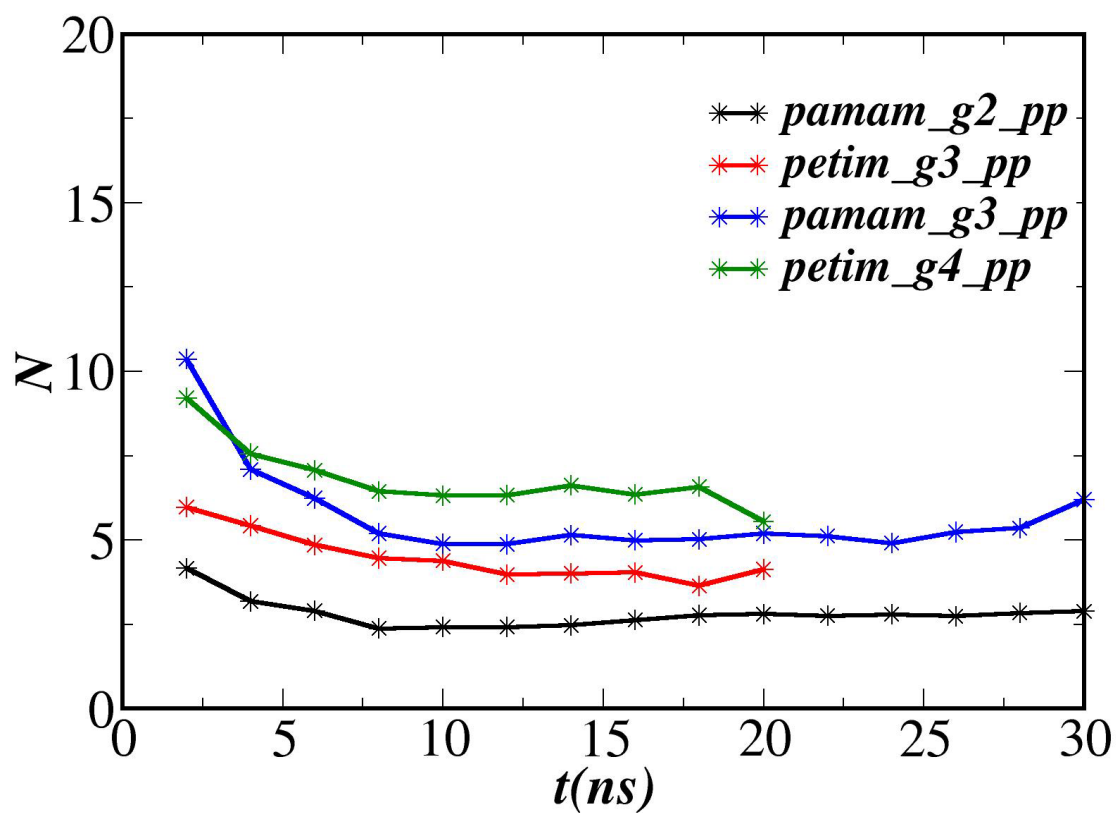


Figure S2: Time variation of the number of Cl⁻ counterions (N) around the dendrimer. For PETIM of generation 3, 4 (within 20 Å) and for PAMAM of generation 2,3 (within 25 Å). Lines are guide to eye only.

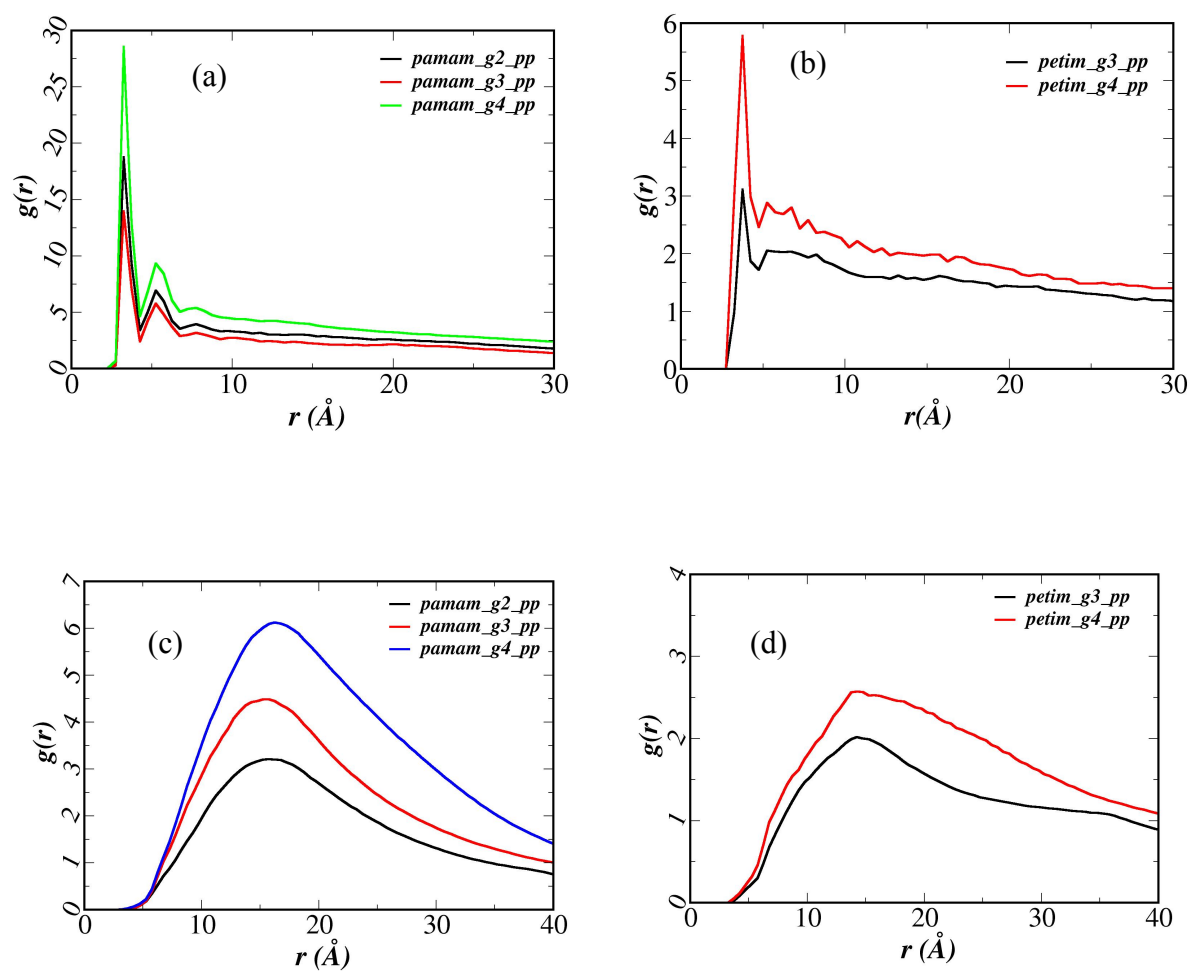


Figure S3: Radial distribution function $g(r)$ of Cl^- from Nitrogen of terminal amines (a) for PAMAM and (b) for PETIM. $g(r)$ of Cl^- from CNT (c) for PAMAM and (d) for PETIM.

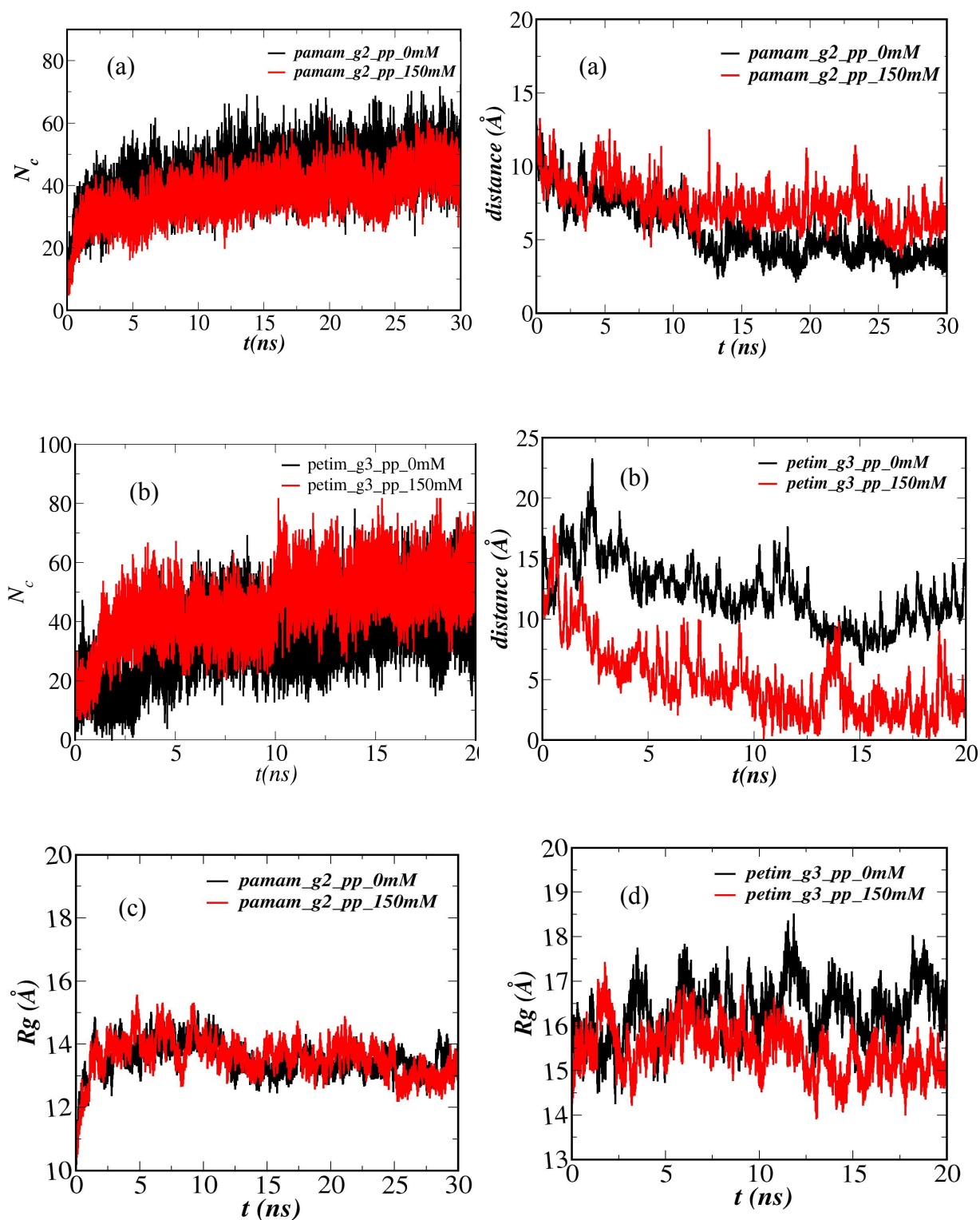


Figure S4: The number of close contacts and COM distance at 0mM and 150mM salt concentrations (a) for protonated PAMAM dendrimer of generation 2 and (b) for protonated PETIM dendrimer of generation 3. The radius of gyration (R_g) of protonated dendrimer at 0mM and 150mM salt concentrations (c) for PAMAM of generation 2 and (d) PETIM of generation 3.

