Supporting Information

pH-dependent conformations for hyperbranched poly(ethyleneimine) from all-atom molecular dynamics

In Kim[†], Tod A. Pascal[‡], Seong-Jik Park[⊥], Mamadou Diallo[†], William A. Goddard III[§], and Yousung Jung[†*]*

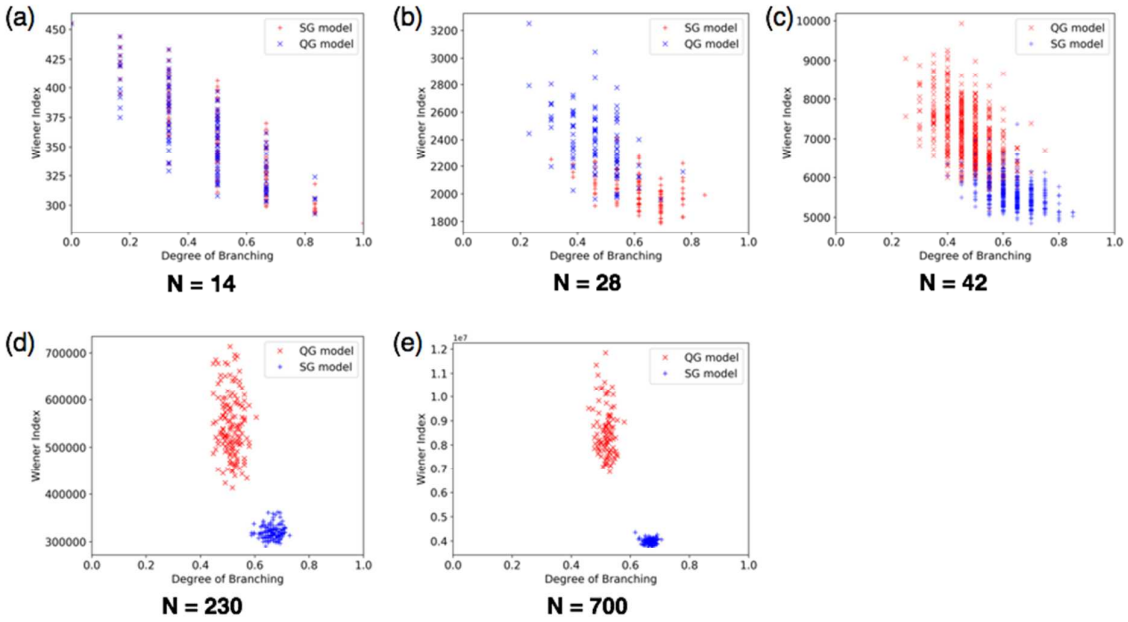

Figure S1. DB values vs. Wiener index from SG and QG growth models. Without applying the attachment probability parameter coarse-grained models with different local structures are obtained from SG and QG methods.

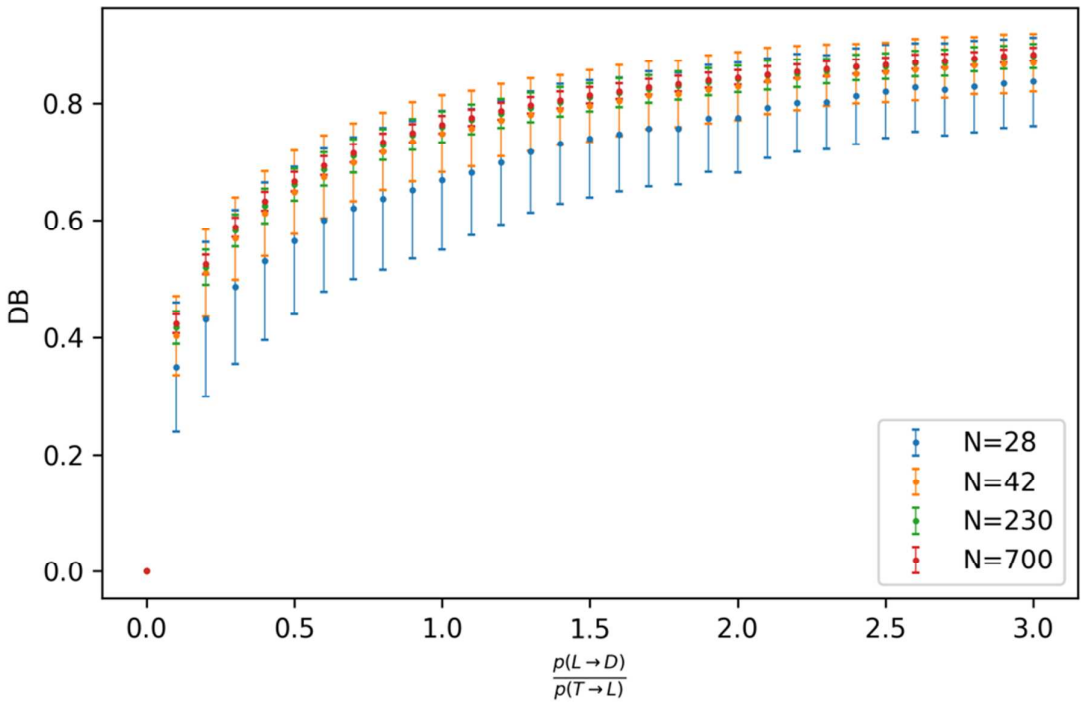

Figure S2. The attachment probability parameter compared to the DB value.

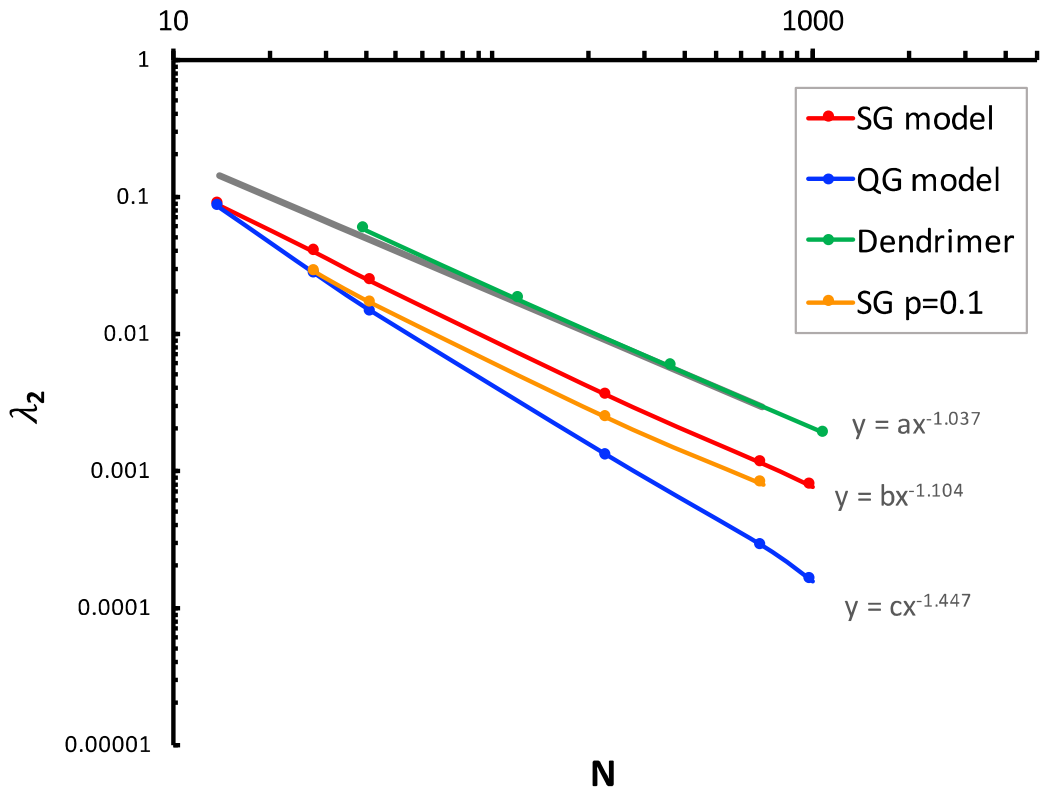

Figure S3. The behavior of the smallest eigenvalue of the connectivity matrix. The black dashed line indicates the slope -1.

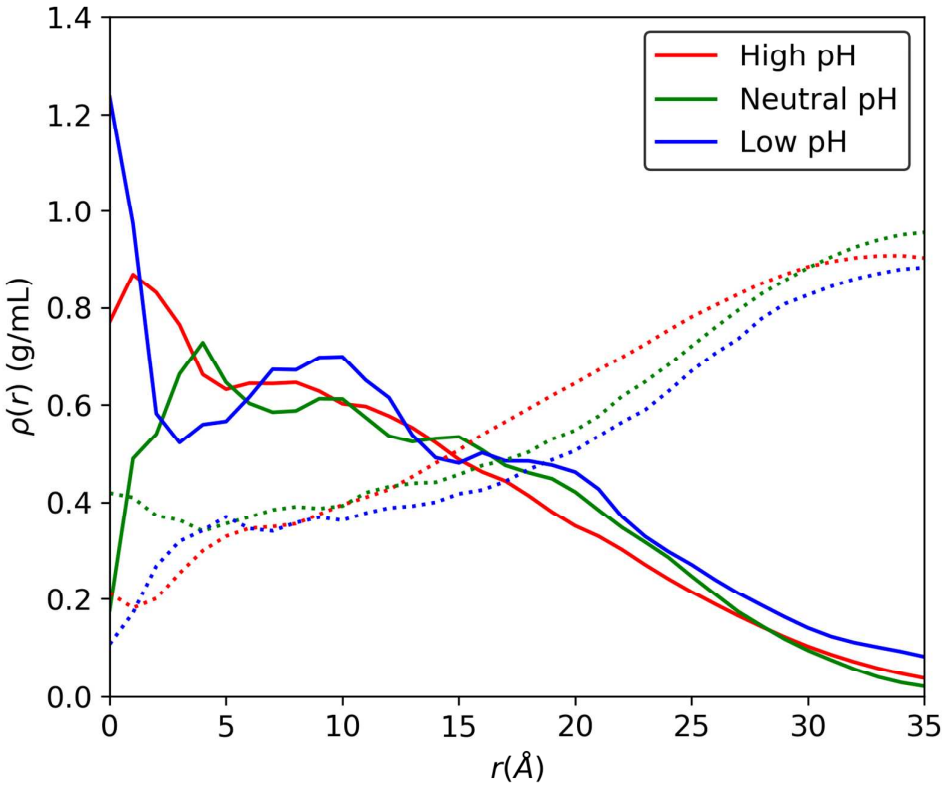

Figure S4. Averaged radial density profiles of all atoms on model hyperbranched PEIs. Solid line, hyperbranched PEI; dashed line, water.

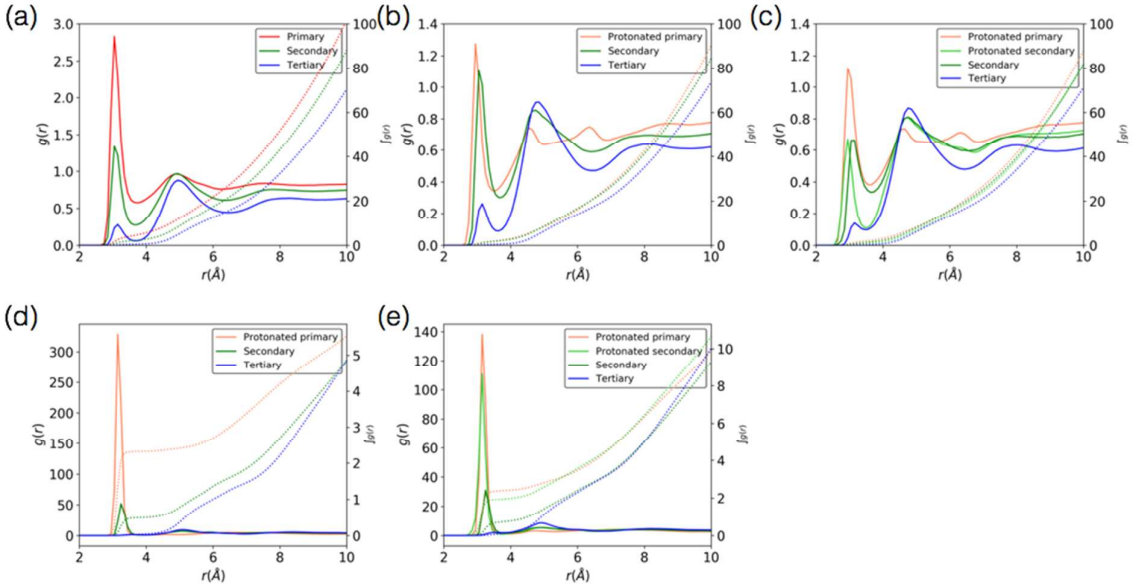

Figure S5. Radial distribution functions for model hyperbranched PEIs between N of PEI and (a) O of water in high pH, (b) O of water in neutral pH, (c) O of water in low pH, (d) Cl^- in neutral pH, (e) Cl^- in low pH condition.

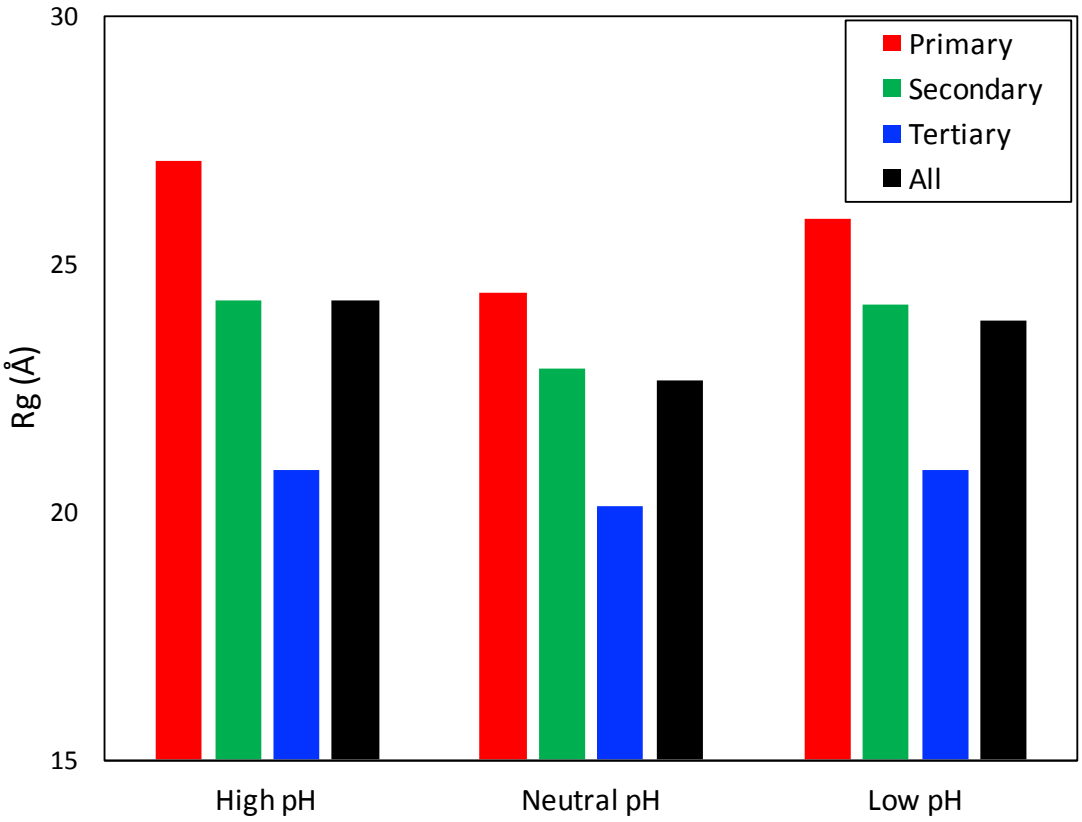

Figure S6. Radius of gyration of the nitrogen atoms in amine groups and all atoms.

Table S1. Solvent accessible surface area (SASA) with probe radius 1.4 Å, and the effective outer radius R_{SASA} of model hyperbranched PEIs at different pH levels.

pH	**SASA (Å^2)**	**R_{SASA} (Å)**
High pH	31970.5	39.2
Neutral pH	30127.0	32.7
Low pH	27179.2	33.4