Conformational dynamics and aggregation behavior of piezoelectric diphenylalanine peptides in an external electric field

Supplementary Material

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Supplementary Material

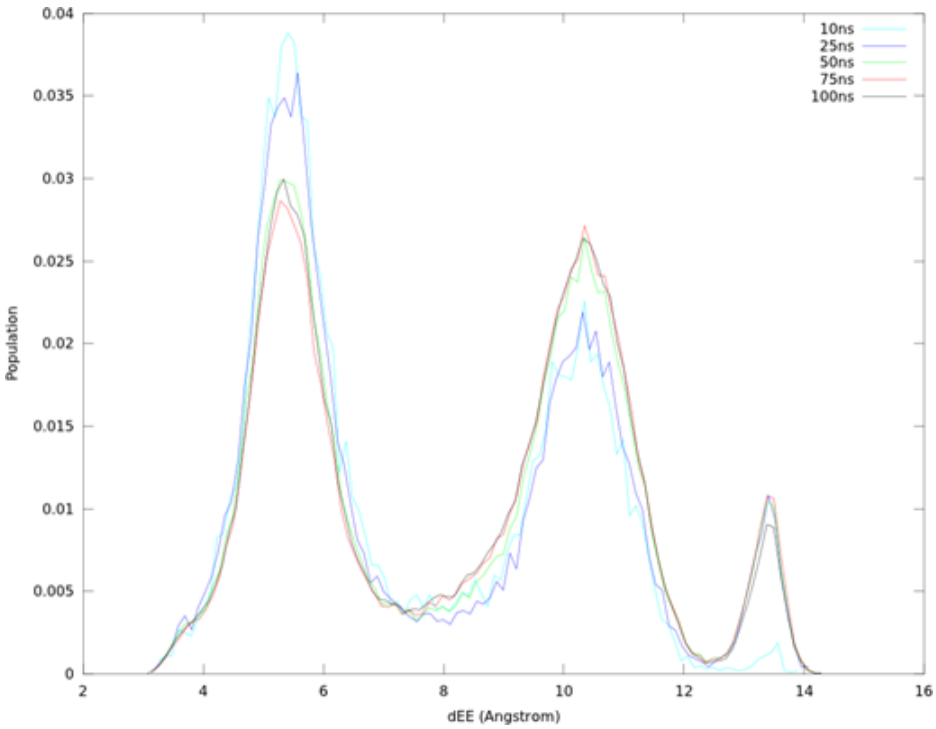

Figure S1. Population distribution of the end-to-end distance, d_{EE}, for the single-FF system with charged termini for different simulation times, 10, 25, 50, 75, 100 ns, showing peak convergence at >50 ns.

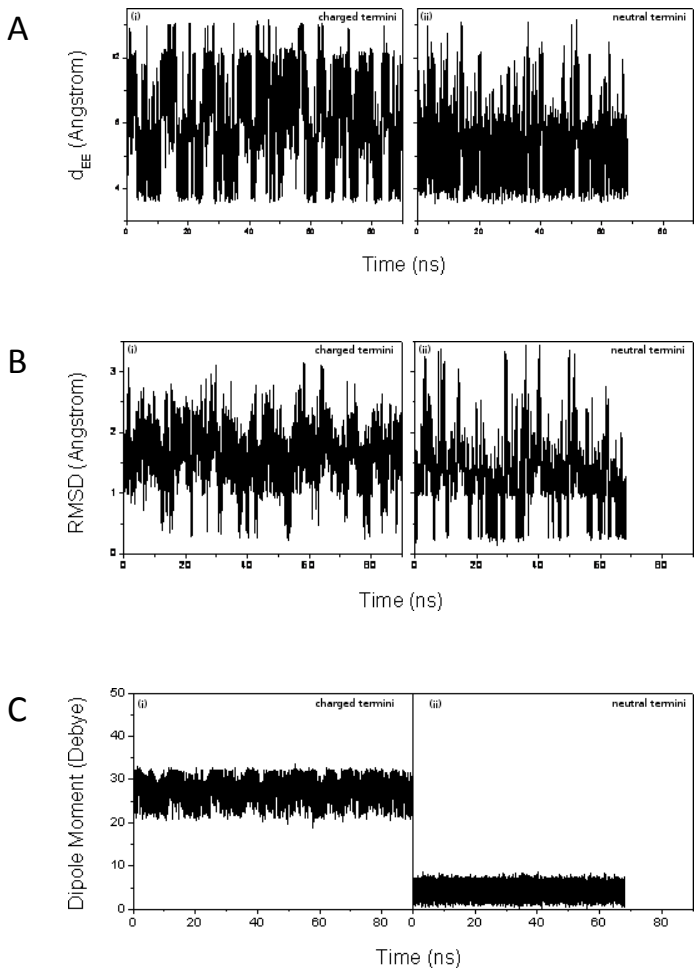

Figure S2. The end-to-end distance, d_{EE}, of the single-FF system with charged termini (A(i)) and neutral termini (A(ii)). RMSDs of non-hydrogen atoms of the single-FF system with respect to its average atomic position with charged termini (B(i)) and with neutral termini (B(ii)). Dipole magnitude over time for the single-FF system with charged (C(i)) and neutral termini (C(ii)).

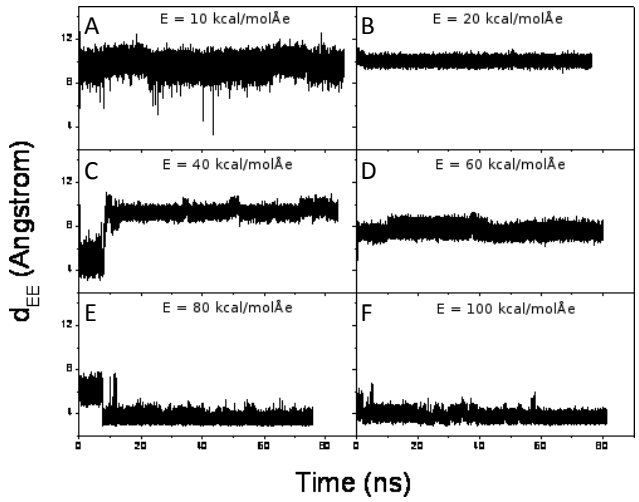

Figure S3. d_{EE} of the single-FF system with field magnitudes E = 10, 20, 40, 60, 80, 100 kcal/(mol Å *e*).

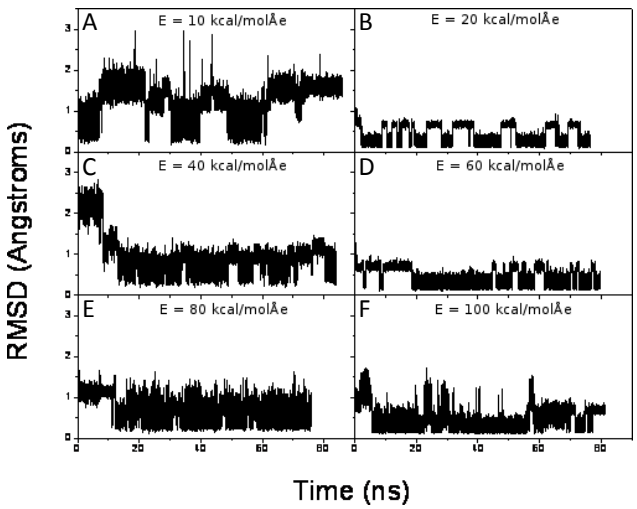

Figure S4. RMSDs with respect to the average position of the non-hydrogen atoms in each case for the charged-termini single-FF system with applied electric field magnitudes 10, 20, 40, 60, 80, 100 kcal/(mol Å *e*).

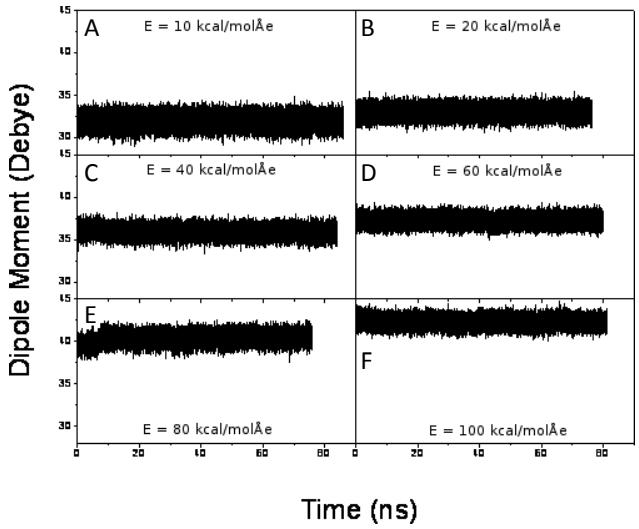

Figure S5. Dipole magnitude for the charged-termini single-FF system for each applied field magnitude E = 10, 20, 40, 60, 80, 100 kcal/(mol Å *e*).