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Article

Effect of Electric Field on α-Synuclein Fibrils: Revealed by Molecular Dynamics Simulations

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Supplementary material

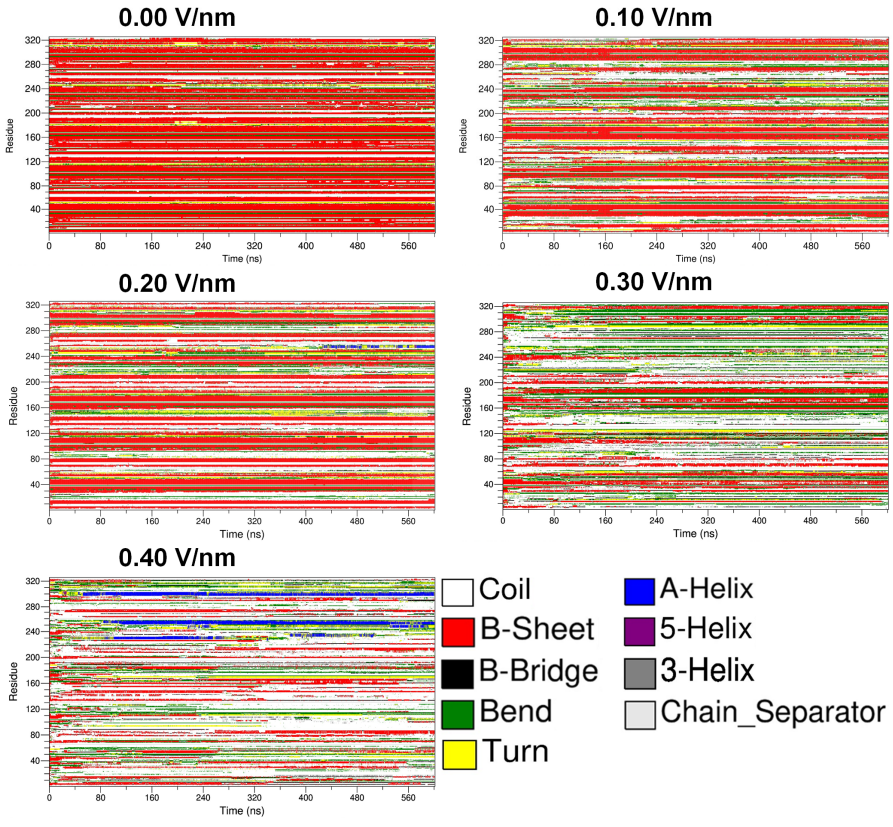


Figure S1. The secondary structure map of α-synuclein fibril under different EF intensities.

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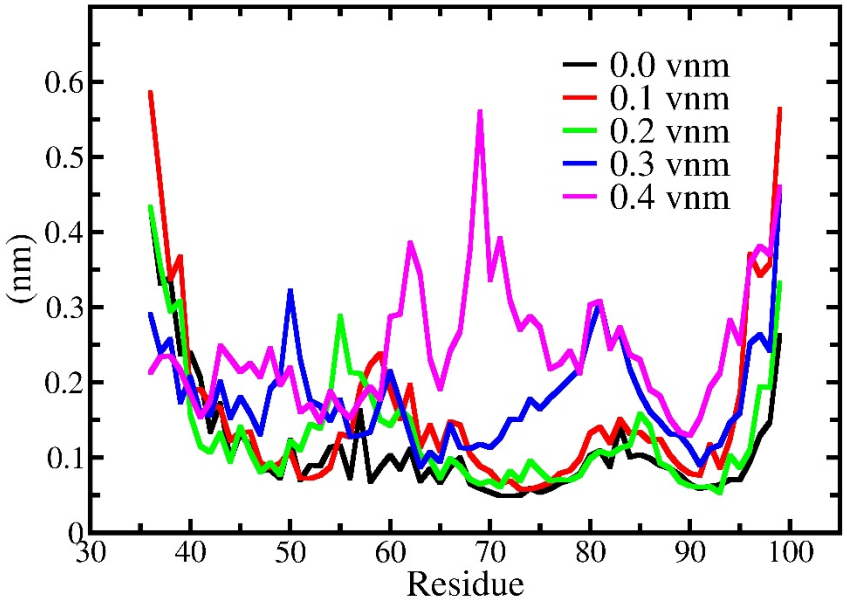


Figure S2. RMSF of chain C influenced by various EF strengths.

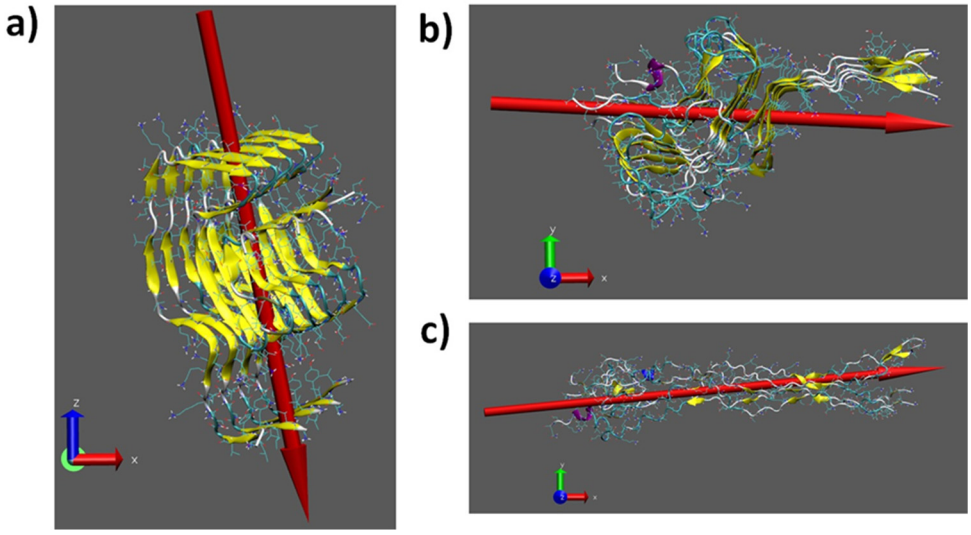


Figure S3. The representation of a total dipole moment of α-synuclein fibril in the case of (**a**) 0 V/nm, (**b**) 0.2 V/nm, and (**c**) 0.4 V/nm.

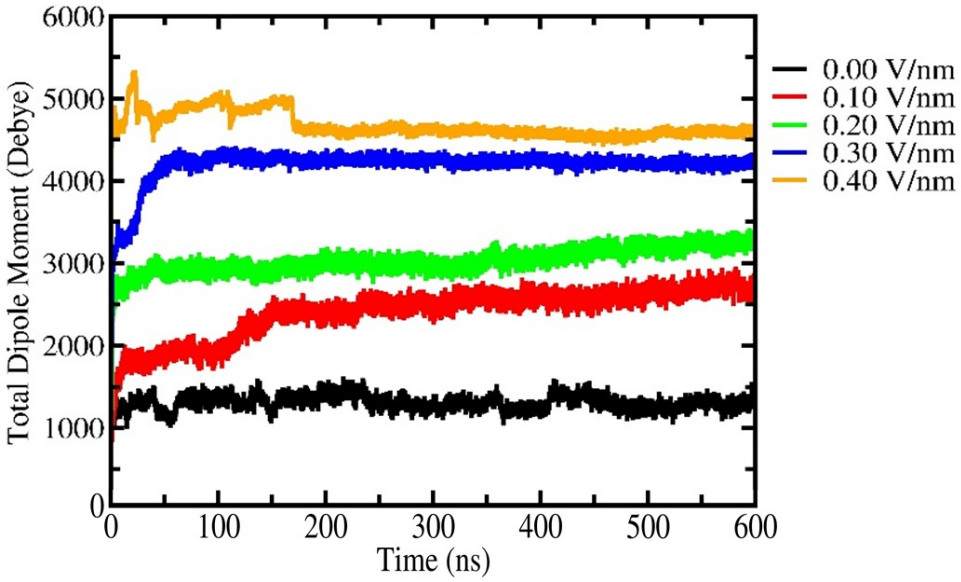


Figure S4. The time evolution of total dipole moment of α-synuclein fibril.

Table S1. The solvent-accessible surface area, the radius of gyration and the number of hydrogen bonds per chain calculated from the last 200 ns of the simulation trajectory for replica 1, 2, 3 and 4.

EF (V/nm)	Rep-lica	SASA (nm^2)	R.Gyration (Å)	h-bond/chain
0.10 M NaCl-neutral model system				
0.00	1	139.58±2.38	2.013±0.02	48.20±1.75
	2	137.95±3.40	2.022±2.66	47.11±2.23
	3	138.08±2.23	2.031±0.01	47.56±1.62
	4	141.36±2.37	2.046±0.01	45.87±2.08
0.05	1	140.52±2.42	2.028±0.01	47.08±1.55
	2	144.47±2.35	2.111±0.01	45.74±1.45
	3	142.73±2.60	2.092±0.02	46.73±1.57
	4	148.04±4.34	2.123±0.03	45.77±1.87
0.10	1	153.90±2.65	2.190±0.01	44,08±1.47
	2	147.47±2.78	2.090±0.01	46.77±1.63
	3	155.85±2.91	2.126±0.01	44.63±1.70
	4	153.41±3.05	2.099±0.01	45.11±1.52
0.15	1	153.27±2.44	2.142±0.01	45.63±1.52
	2	164.00±3.90	2.174±0.02	40.78±1.63
	3	152.16±2.90	2.092±0.01	42.25±1.50
	4	146.09±2.50	2.084±0.01	44.89±1.47
0.20	1	150.69±2.75	2.136±0.01	44.73±1.50
	2	151.32±2.96	2.141±0.01	45.59±1.47
	3	149.20±3.30	2.113±0.02	44.85±1.63
	4	153.92±3.61	2.145±0.01	43.07±1.69
0.25	1	152.02±2.65	2.214±0.01	45.68±1.44

	2	153.56±3.19	2.764±0.02	42.60±1.85
	3	151.39±2.98	2.122±0.01	44.51±1.53
	4	162.47±5.88	2.967±0.02	41.24±1.54
0.30	1	164.08±4.01	3.150±0.03	40.03±1.65
	2	170.90±4.68	3.300±0.03	38.79±1.76
	3	166.89±2.77	2.577±0.02	39.43±1.57
	4	161.30±3.17	2.331±0.01	40.76±1.60
0.35	1	166.54±4.33	3.398±0.02	40.30±1.58
	2	172.34±6.90	4.006±0.03	35.78±2.05
	3	171.71±5.03	2.949±0.03	39.04±1.82
	4	168.14±5.07	3.403±0.02	40.44±1.62
0.40	1	184.36±4.32	4.179±0.02	35.32±1.83
	2	167.69±3.63	3.095±0.05	38.33±1.84
	3	192.05±6.73	4.167±0.02	35.28±1.75
	4	168.07±4.01	4.081±0.01	38.83±1.80
Added counter ion Cl-neutral model system				
0.40	1	163.22±3.12	3.795±0.02	38.68±1.59
	2	177.73±2.75	4.171±0.02	37.74±1.47
	3	172.21±2.36	4.047±0.02	39.29±1.56
	4	177.03±3.85	4.010±0.02	38.42±1.68

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