Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Molecular mechanisms underlying nanowire formation in pristine phthalocyanine

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Table S1: List of different concentrations of phthalocyanine aggregates simulated in terms of number ratios and corresponding molar concentrations.

Number ratio	Concentration (M)
1:50	1106.38
1:60	922.03
1:80	691.46
1:118	468.15
1:125	442.56
1:250	221.28
1:259	213.51
1:817	65.68 (Replicate sets: 4)
1:1069	57.73 (Replicate sets: 4)

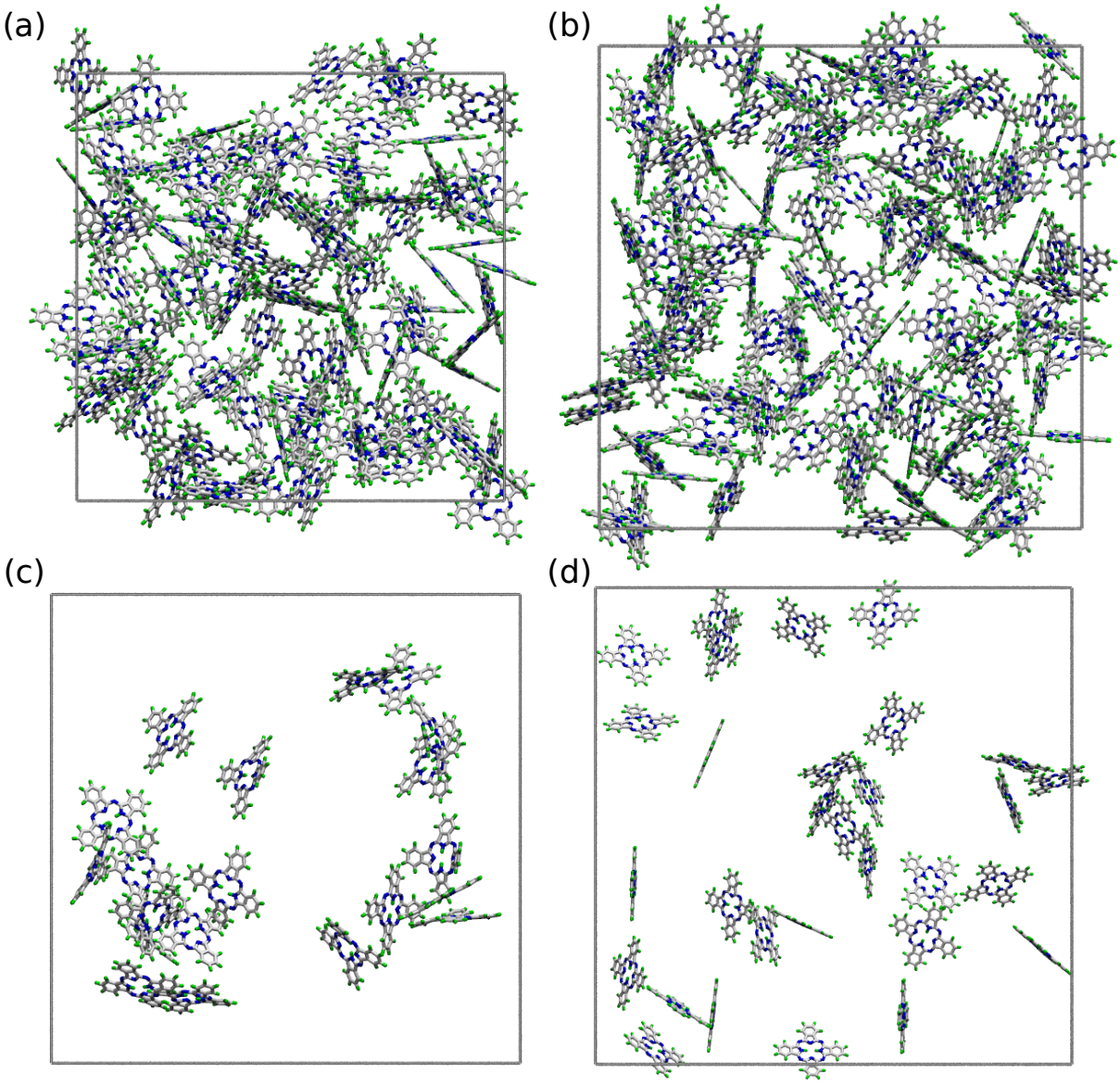

Figure S1: Snapshots of initial random arrangements of phthalocyanine molecules at number ratios (a) 1:60, (b) 1:250, (c) 1:817, (d) 1:1069. The surrounding water molecules are not shown for clarity.

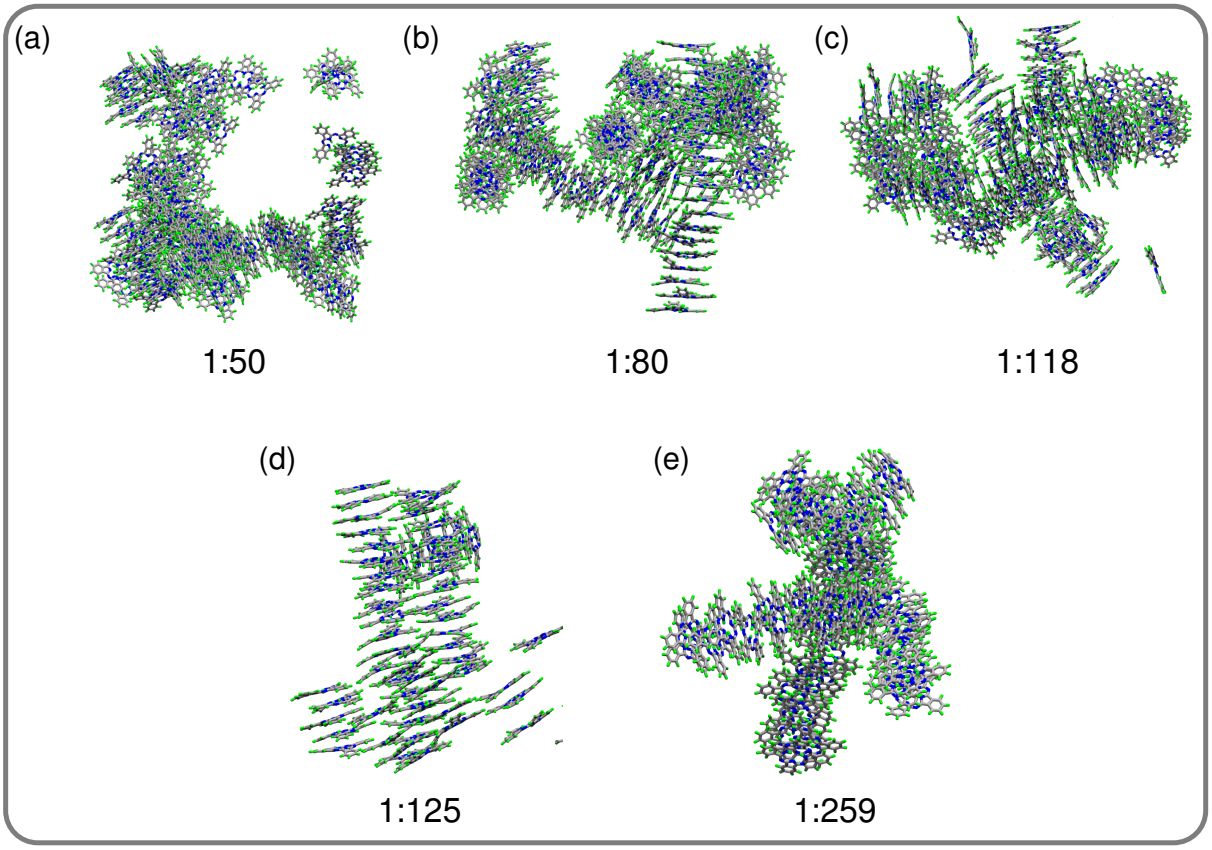

Figure S2: Representative snapshots of phthalocyanine aggregates at number ratios (a) 1:50, (b) 1:80, (c) 1:118, (d) 1:125, (e) 1:259. The surrounding water molecules are not shown for clarity.

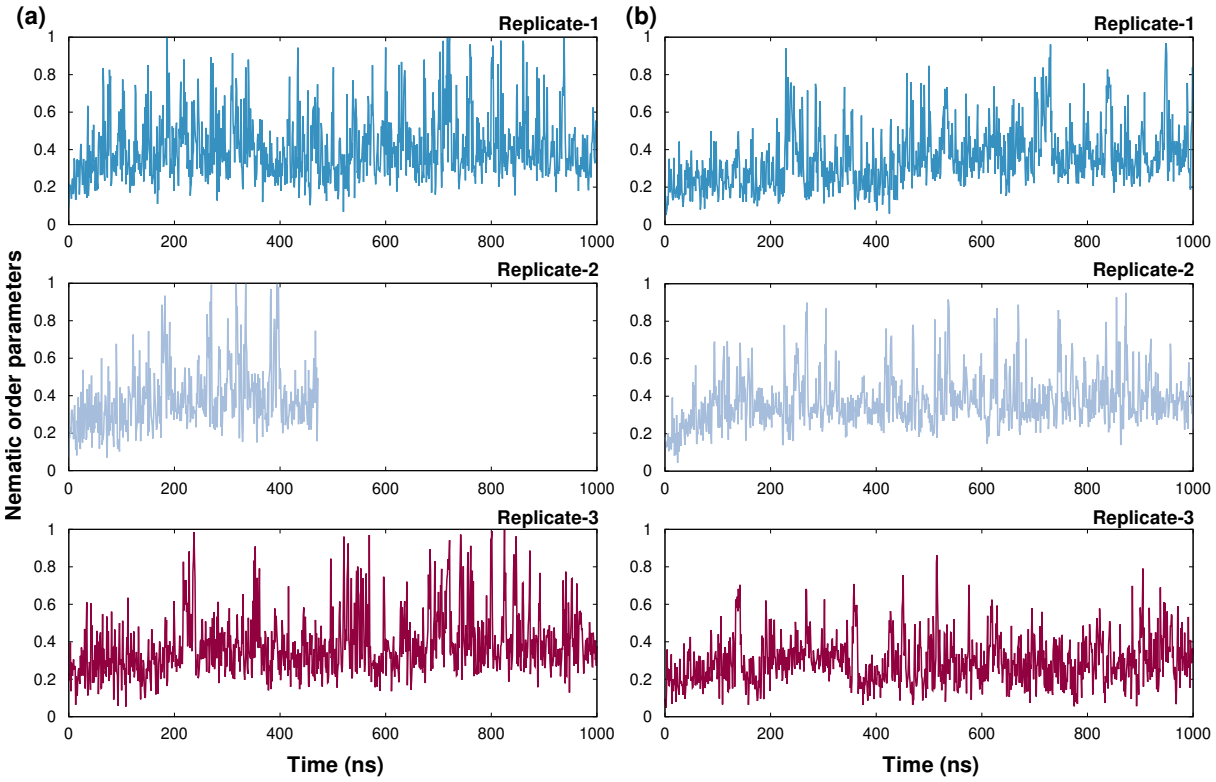

Figure S3: Nematic order parameter of different replicates for number ratios (a) 1:817 and (b) 1:1069.

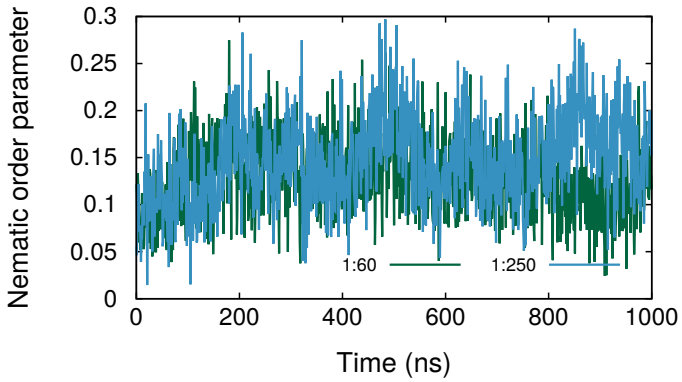

Figure S4: Nematic order parameter for number ratios 1:60 and 1:250.

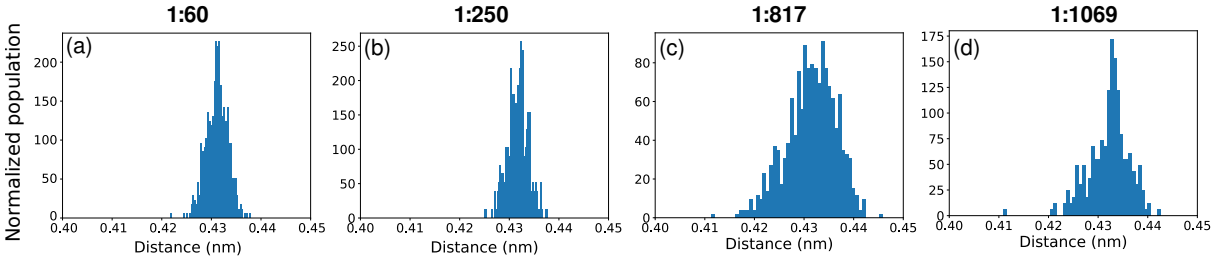

Figure S5: Population histograms of distribution of distances between pairs of neighboring molecules in phthalocyanine self-assemblies of number ratios (a) 1:60, (b) 1:250, (c) 1:817, (d) 1:1069.

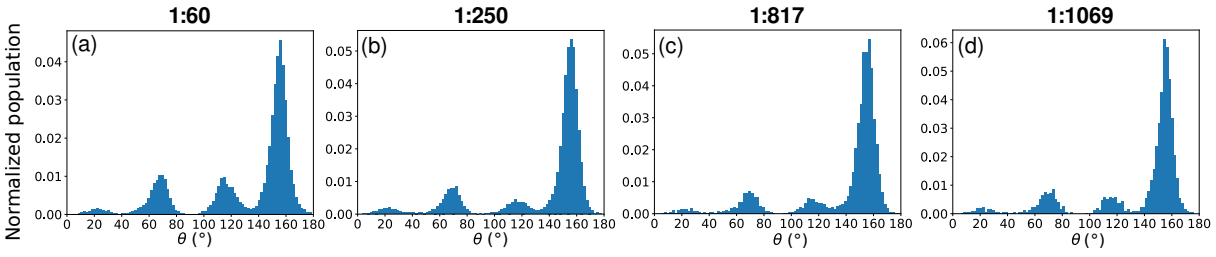

Figure S6: Population histograms of distribution of angles between pairs of neighboring molecules in phthalocyanine self-assemblies at number ratios (a) 1:60, (b) 1:250, (c) 1:817, (d) 1:1069.