Supplement to: Electrostatics and depletion determine competition between 2D nematic and 3D bundled phases of rod-like DNA nanotubes

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S1 DNA sequences

NTs are assembled from six oligos, with lengths and sequences given in Table S1. These six oligos are based on those used by Bertrand *et al.* [1], which in turn was based on sequences developed by Rothemund *et al.* [2]. Note that the naming scheme in Bertrand differs from that used in Rothemund; we refer here to the names used in Bertrand. We use oligos SE1 through SE5 exactly as in Bertrand. The sixth oligo is a truncation of the oligo termed SE6-2 in Bertrand, retaining bases five through thirty. The six oligos assemble into a tile. Tiles assemble into rod-like nanotubes at a density of 7 tiles every 14.5 nm. Given that each tile contains 174 nucleotides, with one charged phosphate per nucleotide, we arrive at a linear charge density of 84/nm, as utilized in the text.

S2 Calculating the effective charge of rods

Our model relies on the calculation of an effective line charge density, ν_{eff}, of the DNA NTs. This permits estimate of rod-rod and rod-plane electrostatic interactions using the formulas of Debye-Huckel solution electrostatics. The method is based on the work of Neukirch and Marko [3] and Stigter [4]. In particular, ν_{eff} is found from Neukirch and Marko's Eq. 1:

$$\nu_{eff} = \frac{\nu \lambda_D}{\gamma r K_1(r/\lambda_D)} \tag{S1}$$

where ν is the actual (bare) line charge density of the rod, λ_D is the solution Debye length, r is the rod radius, K_1 is the 1st modified Bessel function of the second kind, and γ is a numerical correction factor that varies with rod and solution parameters.

The value of γ is found from the numerical results of Stigter [4]. Stigter presents a table (his Table III) of values of γ calculated for a variety of values of the parameters x_0 and y_0, where $x_0 = r/\lambda_D$, $y_0 = e\psi_0/k_BT$, ψ_0 is the potential at the surface of the cylinder, e is the electronic charge, and k_BT is the thermal energy. This table is reproduced here as Table S2.

Knowledge of biomolecular structure and solution conditions gives r, ν, and λ_D, but these do not determine the value of y_0. To find γ, it is necessary to use a second correction parameter, β. β is a numerically-calculated parameter that interrelates x_0 and y_0 through the following equation (Stigter's Eq. 16):

$$\beta y_0 = \frac{2 l_B \nu}{x_0} \frac{K_0(x_0)}{K_1(x_0)}. \tag{S2}$$

Stigter presents a table of values of β for a range of values of x_0 and y_0 (his Table II). However, Eq. S2 shows that the product βy_0 (and not β alone) can be directly calculated from the input parameters (r, ν, λ_D). Thus, a more practically useful table is that of βy_0 as a function of x_0 and y_0; this is presented here as Table S3.

The procedure for finding the effective charge of the rod, given r, ν and λ_D, is then as follows:

1. Calculate $x_0 = r/\lambda_D$
2. Use Eq. S2 to calculate βy_0
3. Using x_0 and βy_0, interpolate in Table S3 to find y_0
4. Using x_0 and y_0, interpolate in Table S2 to find γ
5. Using γ, calculate ν_{eff} using Eq. S1

Here, we carry out interpolation using the Mathematica *Interpolation* function. For step 3, Table S3 is used to construct a first order interpolation function for y_0 over the space $(\log x_0, \beta y_0)$. For step 4, Table S2 is used to construct a second order interpolation function for γ over the space $(\log x_0, y_0)$.

References

[1] O. J. N. Bertrand, D. K. Fygenson and O. A. Saleh, *Proceedings of the National Academy of Sciences of the United States of America*, 2012, **109**, 173427.

[2] P. W. K. Rothemund, A. Ekani-Nkodo, N. Papadakis, A. Kumar, D. K. Fygenson and E. Winfree, *Journal of the American Chemical Society*, 2004, **126**, 1634452.

[3] S. Neukirch and J. F. Marko, *Physical Review Letters*, 2011, **106**, 138104.

[4] D. Stigter, *Journal of Colloid and Interface Science*, 1975, **53**, 296306.

Table S1: Sequences of oligos used to assemble the NTs

oligo name	*length*	*sequence*
SE1	37	`CTC AGT GGA CAG CCG TTC TGG AGC GTT GGA CGA AAC T`
SE2	26	`GTC TGG TAG AGC ACC ACT GAG AGG TA`
SE3	42	`CCA GAA CGG CTG TGG CTA AAC AGT AAC CGA AGC ACC AAC GCT`
SE4	26	`CAG ACA GTT TCG TGG TCA TCG TAC CT`
SE5	17	`CGA TGA CCT GCT TCG GT`
SE6-2_{5-30}	26	`ATG CAC TAC TGT TTA GCC TGC TCT AC`

Table S2: Values of γ calculated by Stigter [4] for values of x_0 ranging from 1/128 to ∞, and values of y_0 ranging from 1 to 8

		y_0							
		1	2	3	4	5	6	7	8
x_0	1/128	1.00274	1.01105	1.02516	1.04543	1.07241	1.1068	1.14944	1.20122
	1/64	1.00341	1.01374	1.03133	1.05671	1.09063	1.13401	1.18785	1.25298
	1/32	1.0043	1.01735	1.03962	1.07185	1.11501	1.1702	1.23834	1.31989
	1/16	1.00549	1.02218	1.0507	1.09198	1.14718	1.21729	1.30282	1.40337
	1/8	1.00706	1.02852	1.06515	1.118	1.18812	1.27601	1.38127	1.50238
	1/4	1.00904	1.03649	1.08311	1.14982	1.23711	1.34455	1.47052	1.61241
	1/2	1.01137	1.04576	1.1037	1.18554	1.2908	1.41779	1.56374	1.72526
	1	1.01383	1.05543	1.1248	1.22136	1.34338	1.488	1.65154	1.83017
	2	1.01609	1.06244	1.14367	1.25274	1.38858	1.54738	1.72492	1.91709
	4	1.01789	1.07112	1.15824	1.27661	1.42249	1.59145	1.77894	1.98073
	8	1.01912	1.07581	1.16805	1.29251	1.44488	1.62036	1.81421	2.02215
	16	1.01986	1.07865	1.17396	1.30203	1.45822	1.63751	1.83508	2.04664
	∞	1.02075	1.08198	1.18083	1.31304	1.47356	1.65719	1.85898	2.07463

Table S3: Values of βy_0, based on Table II of Stigter [4], for values of x_0 ranging from 1/128 to ∞, and values of y_0 ranging from 1 to 8

		y_0							
		1	2	3	4	5	6	7	8
x_0	1/128	1.0014	2.0115	3.04062	4.10276	5.21925	6.4251	7.7805	9.392
	1/64	1.00212	2.01752	3.06246	4.16044	5.34895	6.69228	8.3034	10.3824
	1/32	1.00331	2.02756	3.09939	4.25904	5.57365	7.16034	9.22516	12.1271
	1/16	1.00529	2.04428	3.16119	4.42528	5.9543	7.95366	10.779	15.0347
	1/8	1.00845	2.071	3.2601	4.69116	6.5605	9.20478	13.194	19.4772
	1/4	1.01309	2.11022	3.40467	5.07656	7.42785	10.9653	16.5303	25.5072
	1/2	1.01908	2.16056	3.58848	5.55968	8.49595	13.0925	20.4908	32.5621
	1	1.0256	2.21492	3.78417	6.06528	9.59315	15.2399	24.4319	39.5088
	2	1.03147	2.2633	3.95592	6.5016	10.5249	17.0387	27.6994	45.2245
	4	1.03586	2.29924	4.08186	6.81716	11.1906	18.3117	29.9953	49.2213
	8	1.0387	2.32226	4.16178	7.0156	11.6057	19.1005	31.4117	51.6791
	16	1.04034	2.33558	4.20768	7.12884	11.8415	19.5468	32.2109	53.0662
	Infinity	1.04219	2.3504	4.25856	7.25372	12.1004	20.0357	33.0852	54.5798