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

Supplementary Information: Photo-phoretic Separation of Single-Walled Carbon Nanotubes: A Novel Approach to Selective Chiral Sorting

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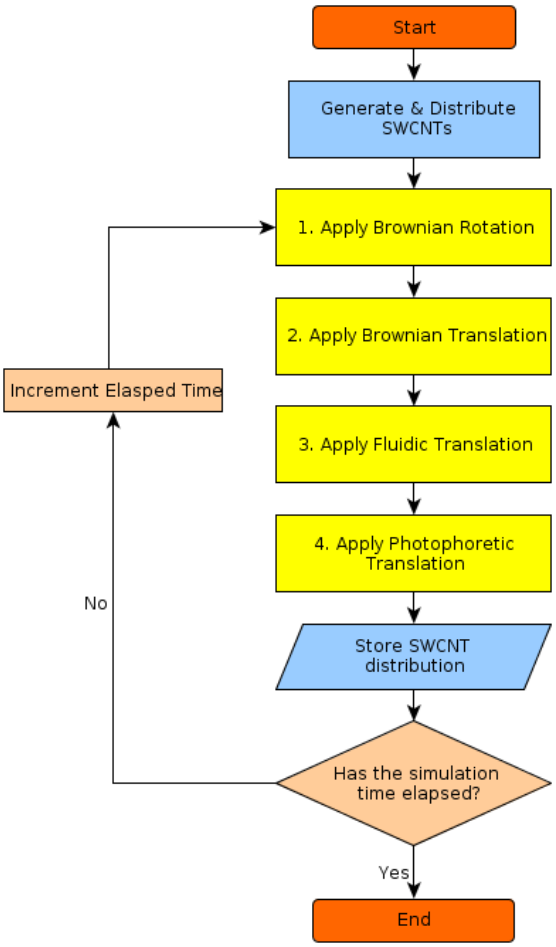

Figure S1: Schematic of simulation steps for chiral separation of SWCNTs. SWCNT are initially generated and distributed across all cores. All SWCNTs are then allowed to evolve within an iterative loop with each iteration simulating a 1ms time step. Each iteration cyclically apply Brownian movement, fluidic translation and photonic translation. This continues to run until the desired simulation time has been modeled. Every 54,000 cycles (54 simulated seconds) the SWCNT are gathered to a single core and their position is stored. This results in 200 data points for every 180 minute simulation.

Parameter	Value
Time Step	*1 ms*
Run Time	*180 minutes*
SWCNT length	*2 μm*
SWCNT diameter	*1 nm*
Surfactant tail length	*0.6 nm*
Absorption Ratio (τ)	*2*

Table S1: The general parameters used in all simulations

$$\eta = \frac{1.79 - 5.90 \times 10^{-2} t + 1.29 \times 10^{-3} t^2 + 1.76 \times 10^{-2} t^3 + 1.30 \times 10^{-7} t^4 - 3.92. \times 10^{-10} t^5}{1000}$$

Equation S1: Empirical relationship between temperature and hydrodynamic viscosity. η is the hydro-dynamic viscosity in N s m^{-2} and t is the temperature in ºc.

Temperature - ºc	Viscosity - mN s m^{-2}
0	1.79
10	1.31
20	1.00
30	0.80
40	0.65
50	0.55
60	0.47
70	0.40
80	0.35
90	0.31
100	0.27

Table S2: Calculated hydrodynamic viscosities at different temperatures

Example S3: A worked example of a single calculation

Worked example for an un-rotating (8,6) chirality SWCNT at an RPI of 1.0 lying at 45 degrees to the Z-axis in the XZ plane at room temperature

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BROWNIAN CALCULATIONS

Unit Vector =
[0.70710678 0. 0.70710678] i.e. lying at 45 degrees in the XZ plane

Unit Tensor =
[[0.5 0. 0.5]
 [0. 0. 0.]
 [0.5 0. 0.5]]

Friction Tensor (kg/s) =
[[2.59924080e-09 0.00000000e+00 -8.66413601e-10]
 [0.00000000e+00 3.46565440e-09 0.00000000e+00]
 [-8.66413601e-10 0.00000000e+00 2.59924080e-09]]

Inverse Friction Tensor (s/kg) =
[[4.32818690e+08 0.00000000e+00 1.44272897e+08]
 [0.00000000e+00 2.88545794e+08 0.00000000e+00]
 [1.44272897e+08 0.00000000e+00 4.32818690e+08]]

Eigenvalues = [5.77091587e+08 2.88545794e+08 2.88545794e+08]

& the corresponding orthogonal Eigenvectors (one per row) =
[[0.70710678 0. 0.70710678]
 [-0.70710678 0. 0.70710678]
 [0. 1. 0.]]
NOTE: Above - The first Eigenvector is parallel to the SWCNT axis the other two are orthogonal

Inverse Friction Coefficients [X,Y,Z] (s/kg) =
[4.56230958e+08 2.88545794e+08 4.56230958e+08]

Diffusion Coefficients [X,Y,Z] (m^2/s) = [1.84472426e-12 1.16670606e-12 1.84472426e-12]

Brownian Standard Deviation [X,Y,Z] (m/s^0.5) = [1.92079372e-06 1.52755102e-06
1.92079372e-06] Brownian Variance [X,Y,Z] (m^2/s) = [3.68944851e-12 2.33341212e-12
3.68944851e-12]

OPTICAL CALCULATIONS

Optical Intensity = 50000000.0 Saturation Intensity = 50000000.0 RPI = 1.0
Optical-cross section (m^2) = 2.44306037589e-15

On Resonance Imparted Momemtum Rate (kg.m/s) = 4.07176729314e-16

On Resonance Drift Velocity (m/s) = 1.85766629479e-07

Off Resonance Imparted Momemtum Rate (kg.m/s) = 2.03588364657e-16
Off Resonance Drift Velocity (m/s) = 9.28833147397e-08

Relative Drift Velocity (m/s) = + 9.28833147397e-08

ESTIMATING THE 2-SIGMA SEPERATION TIME

2-Sigma Separation occurs when the difference in the mean positions (relative velocity (Vrel) * Time) is equal to 4 Standard Deviations (2 contributed by each population)
i.e Vrel * t = 4 SD(t)
given that SD(t)^2 = Variance * t
then the 2-Sigma Separation Time if found by

Tsep = 16 * Brownian Variance / Vrel^2

Therefore at an RPI of 1.0 at room temperature we estimate the separation time to be:

2-Sigma Separation Time (minutes) = 114 minutes

As mentioned above merely assuming the ' rate proportional to the intensity' is overly simplistic due to saturation effects.