

Nanoparticle Metrology of Silicates Using Time-Resolved Multiplexed Dye Fluorescence Anisotropy, Small Angle X-ray Scattering, and Molecular Dynamics Simulations

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Supplementary Information

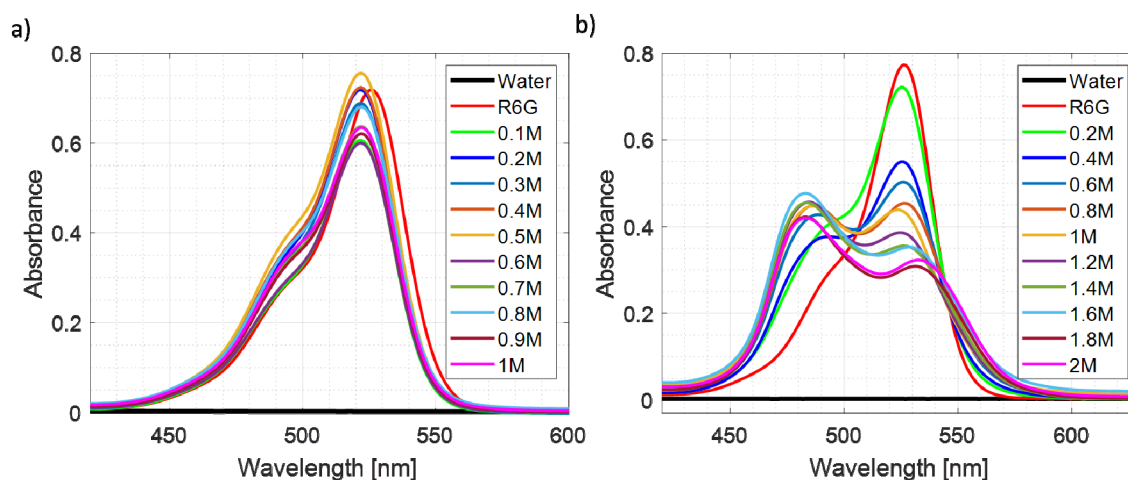


Figure S1. UV-Vis absorption Spectra of (a) R6G at different concentrations of NaOH; (b) R6G in Sodium silicate containing different concentrations of NaOH.

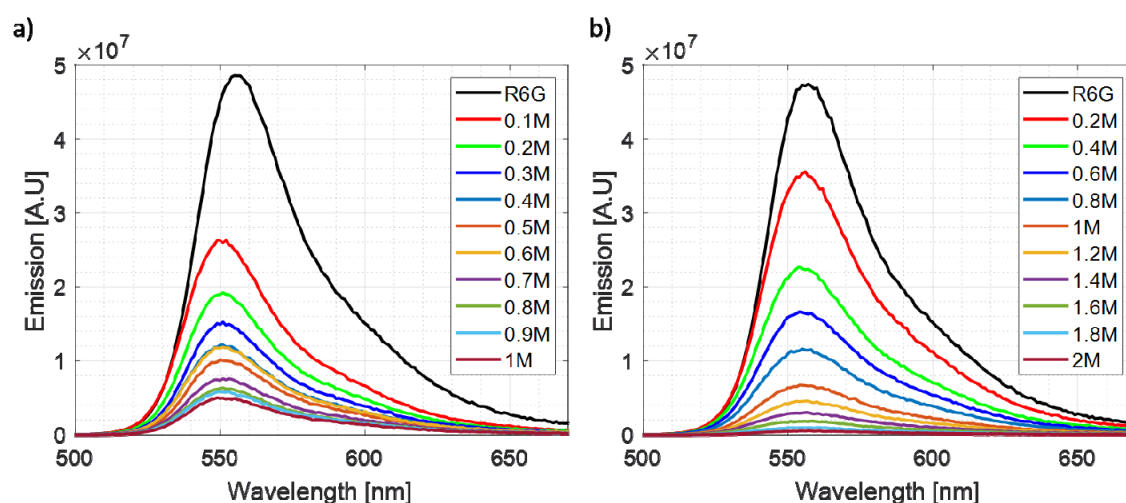


Figure S2. Emission Spectra ($\lambda_{ex}=494$ nm) of (a) R6G at different concentrations of NaOH; (b) R6G in Sodium silicate containing different concentrations of NaOH.

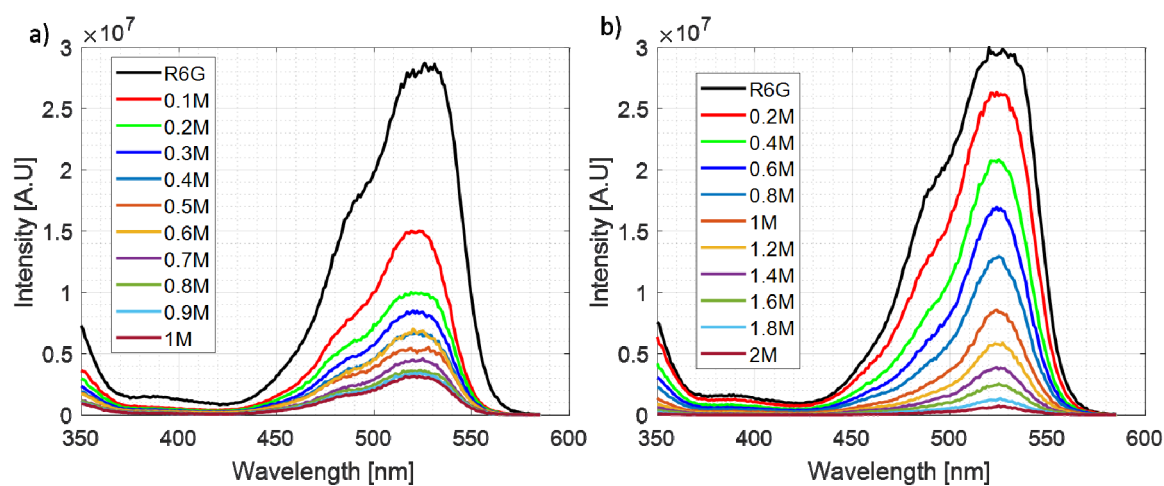


Figure S3. Excitation Spectra ($\lambda_{em}=590$ nm) of (a) R6G at different concentrations of NaOH; (b) R6G in Sodium silicate containing different concentrations of NaOH.

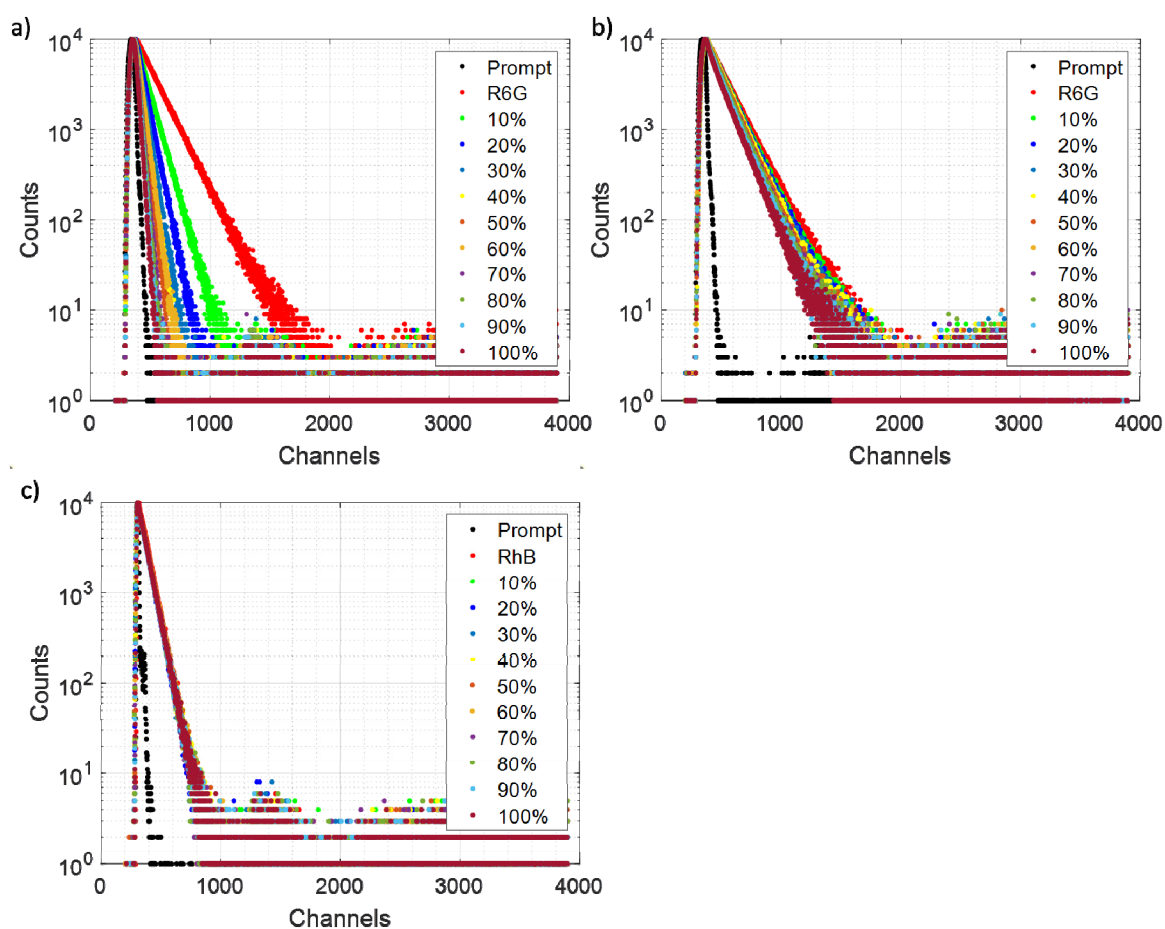


Figure S4. Fluorescence intensity decays of (a) R6G in NaOH, (b) R6G-silicate complex; (c) RB in sodium silicate.

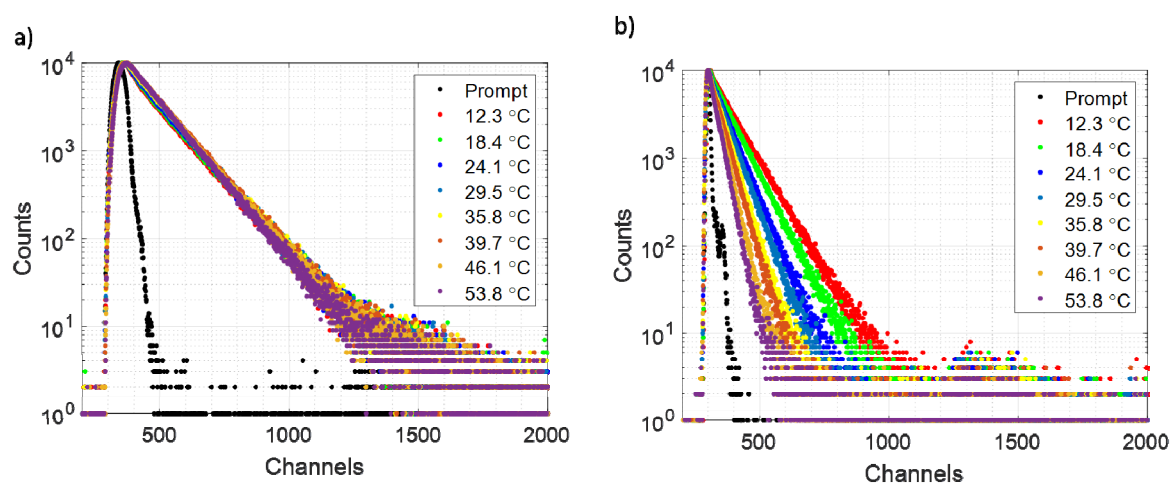


Figure S5. Fluorescence intensity decays at different temperatures (a) R6G-Silicate complex; (b) RB in Sodium Silicate.

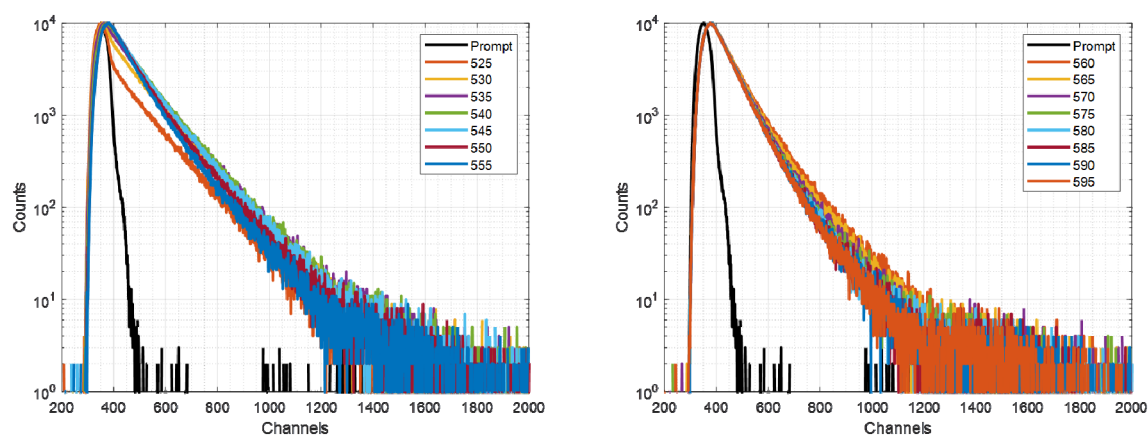


Figure S6. Fluorescence intensity decays for the multiplexed measurements.

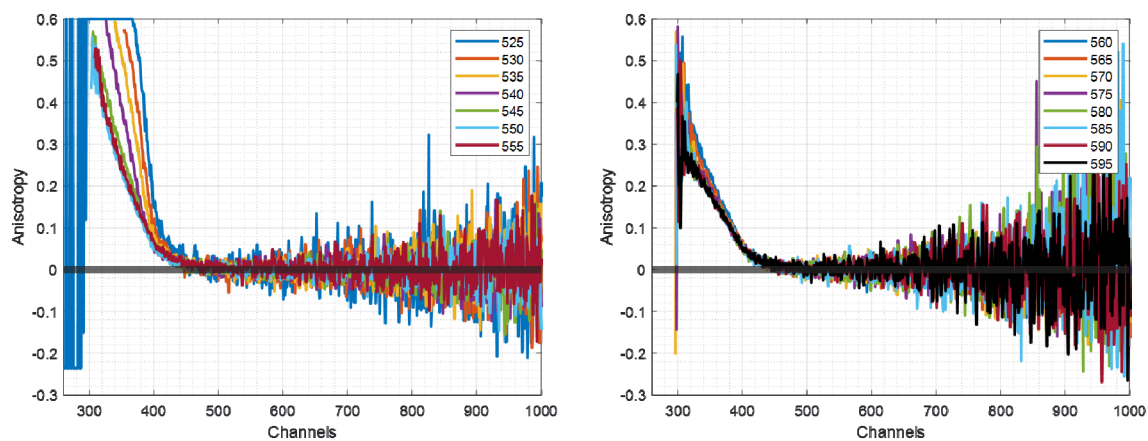


Figure S7. Anisotropy decays for the multiplexed measurements.

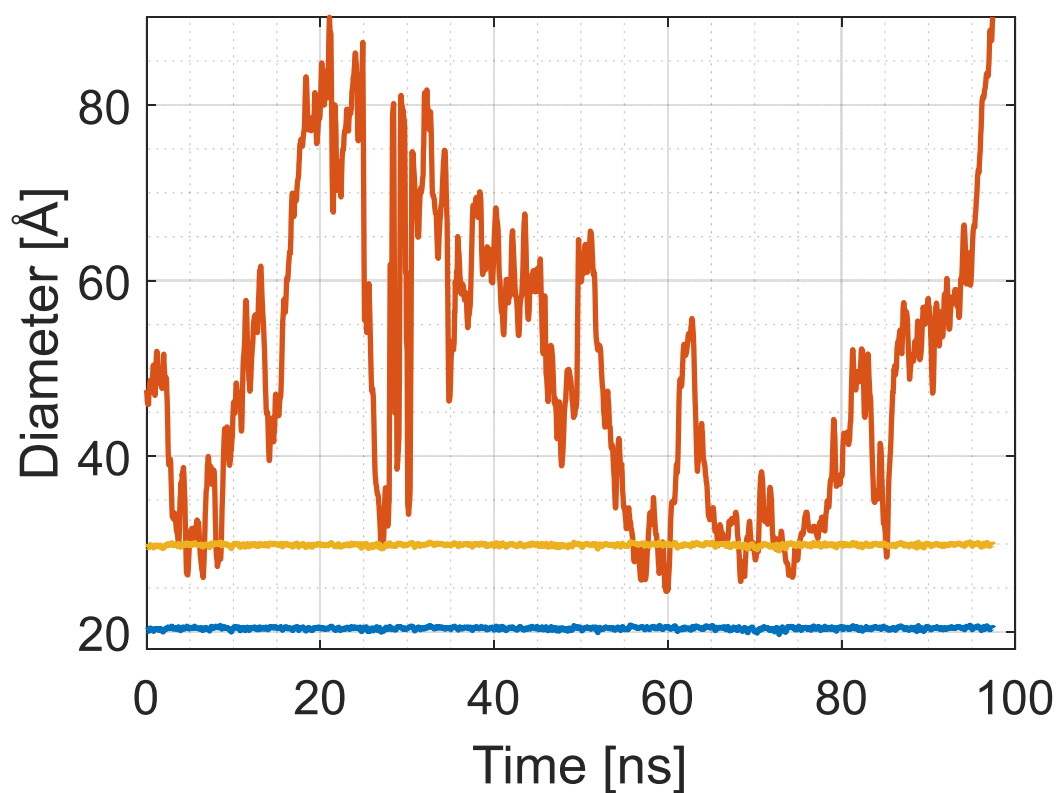


Figure S8. 20 Å diameter SNP measurement results. Colour code follows the one introduced on Figure 9 while the sum of separated sizes is ignored for clarity.

Table S1. R6G Parameters recovered from Fluorescence Intensity Decay fitting.

SiO ₂ (%)	[NaOH] M	T1 (ns)	B1 (%)	T2 (ns)	B2 (%)	C (%)	X ²
27.0	2.0	3.42	82.43	0.94	8.01	9.56	1.23
24.3	1.8	3.46	88.30	0.79	5.19	6.50	1.13
21.6	1.6	3.51	93.43	0.58	3.43	3.14	1.18
18.9	1.4	3.55	93.06	0.57	3.59	3.35	1.12
16.2	1.2	3.55	95.23	0.45	3.63	1.15	1.05
13.5	1.0	3.65	94.19	0.59	2.16	3.65	1.09
10.8	0.8	3.73	93.98	0.69	1.14	4.58	1.16
8.1	0.6	3.81	93.39	1.43	1.66	4.95	1.19
5.4	0.4	3.89	93.58	1.78	2.53	3.89	1.18
2.7	0.2	3.98	95.87	0.61	1.40	2.73	1.13
0.0	0.0	4.18	97.20	-	-	2.80	1.07

Table S2. RhB Parameters recovered from Fluorescence Intensity Decay Fitting.

SiO ₂ (%)	[NaOH] M	T1 (ns)	B1 (%)	T2 (ns)	B2 (%)	C (%)	χ ²
27.0	2.0	1.69	90.62	0.38	5.62	3.76	0.97
24.3	1.8	1.70	90.25	0.38	5.94	3.81	1.08
21.6	1.6	1.69	92.47	0.24	4.58	2.94	1.04
18.9	1.4	1.69	91.54	0.31	5.36	3.09	0.99
16.2	1.2	1.72	93.32	0.22	3.23	3.45	1.08
13.5	1.0	1.71	94.33	0.30	2.12	3.55	1.04
10.8	0.8	1.73	92.31	0.33	3.78	3.91	1.13
8.1	0.6	1.69	93.84	0.16	2.78	3.38	1.17
5.4	0.4	1.65	93.85	0.22	1.87	4.28	1.16
2.7	0.2	1.68	94.49	0.18	2.03	3.48	0.97
0.0	0.0	1.67	94.15	0.17	2.78	3.06	0.95

Table S3. Anisotropy Fitting Results for R6G-Silicate complex.

SiO ₂ (%)	[NaOH] M	Φ (ns)	R0	χ ²
27.0	2.0	1.16	0.17	1.10
24.3	1.8	0.84	0.13	1.10
21.6	1.6	0.40	0.31	1.11
18.9	1.4	0.44	0.21	1.05
16.2	1.2	0.27	0.29	1.07
13.5	1.0	0.19	0.33	1.26
10.8	0.8	0.24	0.28	1.08
8.1	0.6	0.17	0.34	1.18
5.4	0.4	0.19	0.22	1.19
2.7	0.2	0.14	0.35	1.12
0.0	0.0	0.16	0.20	1.06

Table S4. Anisotropy Fitting Results for RhB in Sodium Silicates.

SiO ₂ (%)	[NaOH] M	Φ (ns)	R0	χ ²
27.0	2.0	0.54	0.17	1.00
24.3	1.8	0.46	0.19	1.00
21.6	1.6	0.41	0.20	1.07
18.9	1.4	0.35	0.20	0.96
16.2	1.2	0.32	0.18	1.02
13.5	1.0	0.40	0.15	1.14
10.8	0.8	0.30	0.18	1.22
8.1	0.6	0.25	0.21	1.03
5.4	0.4	0.26	0.15	1.07
2.7	0.2	0.22	0.16	1.19
0.0	0.0	0.22	0.22	1.01

Table S5. R6G Parameters recovered from Fluorescence Intensity Decay fitting.

T (°C)	T1 (ns)	B1 (%)	T2 (ns)	B2 (%)	C (%)	χ²
12	3.47	75.88	1.01	10.73	10.72	1.19
18	3.45	81.34	0.89	9.40	9.27	1.29
24	3.42	84.90	0.82	6.30	8.80	1.20
29	3.41	86.69	0.96	5.31	8.00	1.21
35	3.35	89.23	0.95	3.01	7.75	1.23
39	3.33	90.74	1.16	3.06	6.21	1.18
46	3.22	92.52	0.88	2.09	5.38	1.15
53	3.11	94.46	-	-	5.54	1.18

Table S6. RB Parameters recovered from Fluorescence Intensity Decay fitting.

T (°C)	T1 (ns)	B1 (%)	T2 (ns)	B2 (%)	C (%)	χ²
12	2.25	87.51	0.59	8.73	3.76	1.07
18	1.93	88.01	0.48	8.04	3.94	0.98
24	1.56	88.30	0.35	6.73	4.97	1.19
29	1.39	87.98	0.33	5.88	6.14	1.01
35	1.15	87.13	0.27	6.85	6.02	1.24
39	1.06	82.52	0.43	9.18	8.30	1.21
46	0.90	68.53	0.47	19.91	11.57	1.09
53	1.13	7.51	0.65	79.36	13.14	1.25

Table S7. Anisotropy Fitting Results for R6G-Silicate Complex.

T (°C)	Φ (ns)	R0	χ²
12	1.17	0.17	1.11
18	0.76	0.13	1.06
24	0.82	0.10	1.09
29	0.51	0.15	1.05
35	0.44	0.17	1.14
39	0.32	0.22	1.05
46	0.18	0.34	1.10
53	0.22	0.25	1.05

Table S8. Anisotropy Fitting Results for RhB in Sodium Silicate.

T (°C)	Φ (ns)	R0	χ²
12	0.72	0.17	1.15
18	0.53	0.17	1.12
24	0.54	0.12	1.10
29	0.37	0.13	1.12
35	0.23	0.12	1.16
39	0.29	0.11	1.15
46	0.19	0.10	1.18
53	0.14	0.09	1.16