

Supporting Information

Not All Silicon Quantum Dots are Equal: Photostability of Silicon Quantum Dots with and without Thick Amorphous Shell

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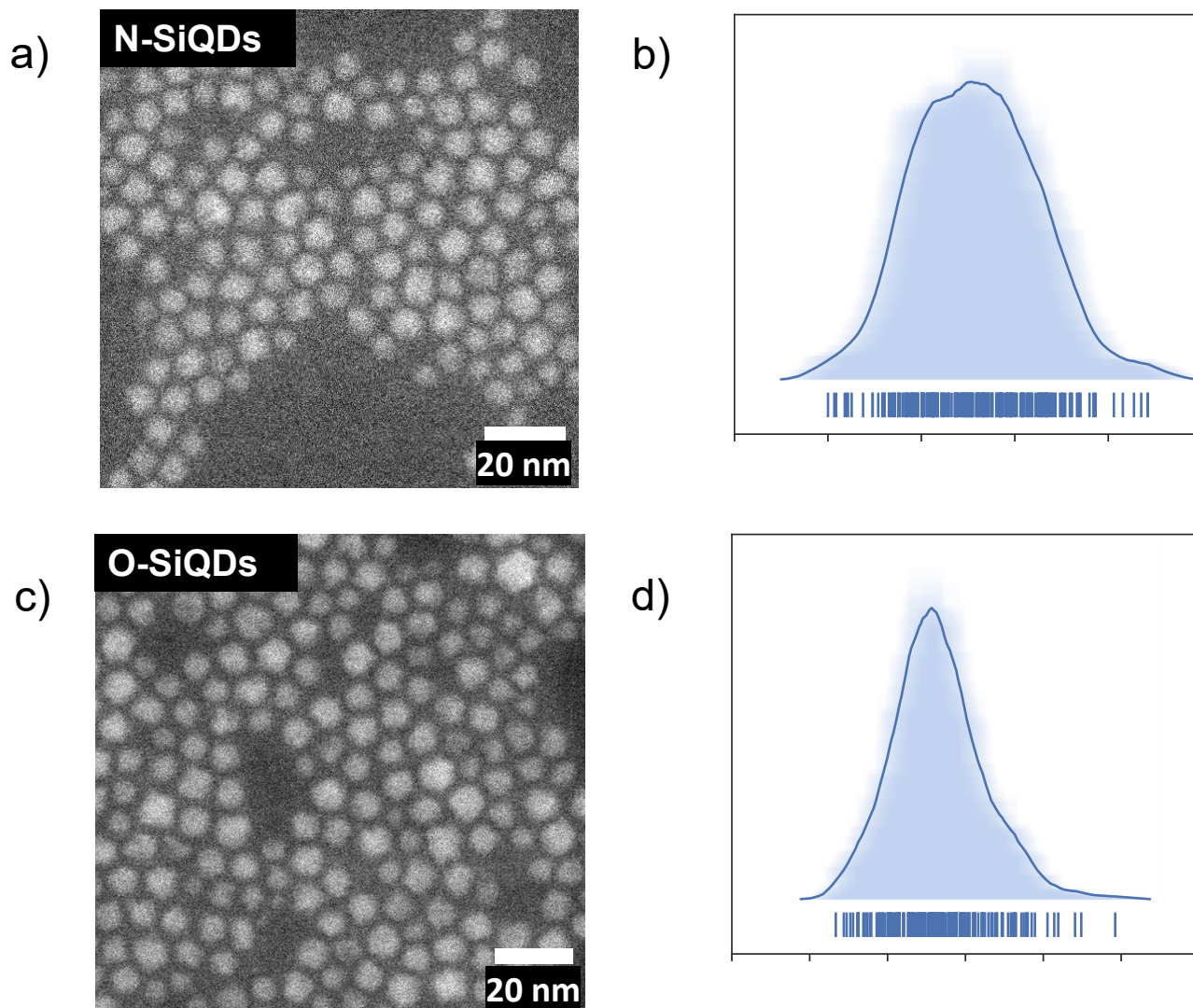


Figure S1. Dark-field TEM images of a) N-SiQDs and c) O-SiQDs. Average-shifted histogram showing the size distribution of as-produced b) N-SiQDs and d) O-SiQDs from corresponding TEM images.

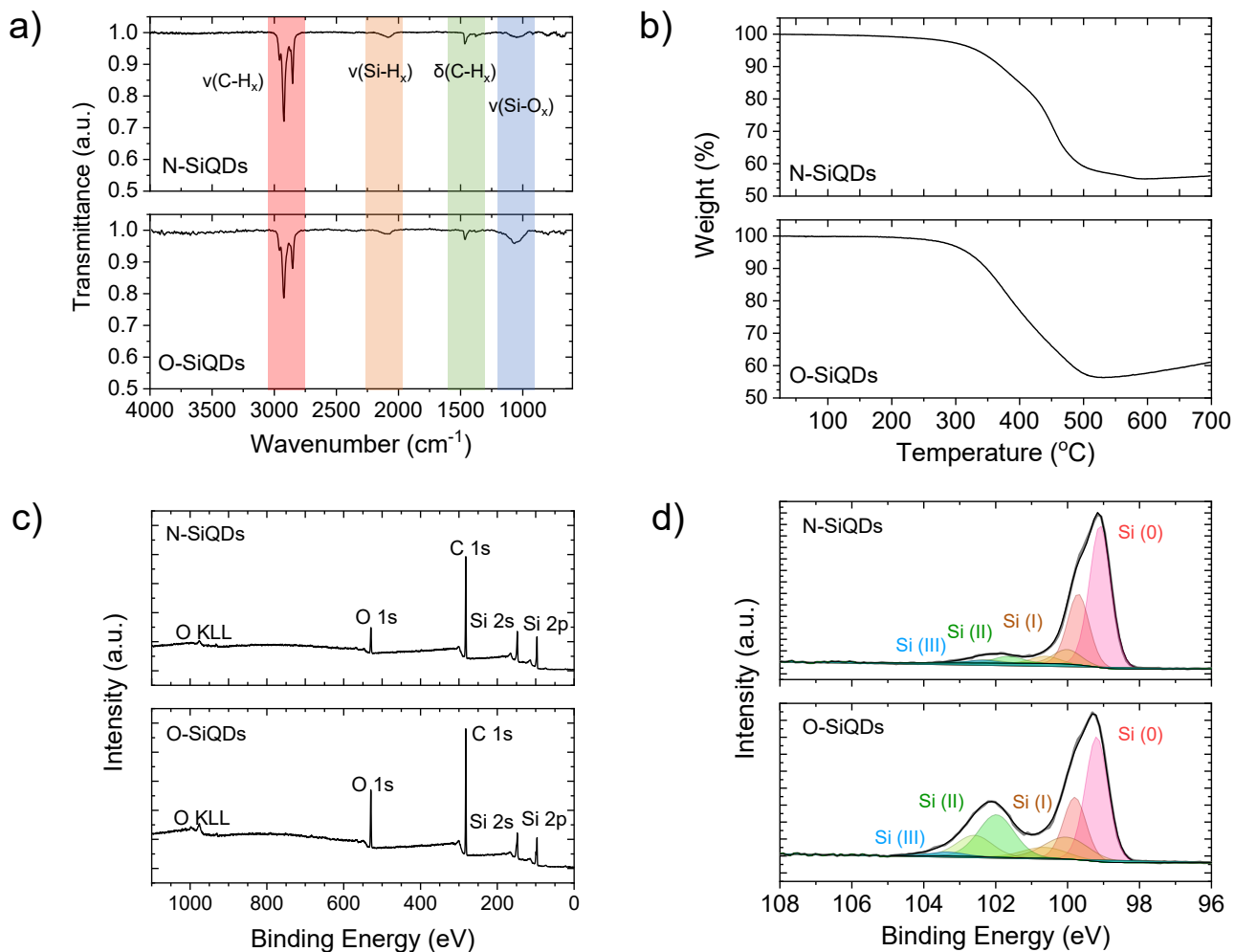


Figure S2. Compositional analyses of the as-produced SiQDs. a) FT-IR spectra and b) TGA of the SiQDs. c) Survey and d) high-resolution Si 2p XPS spectra of the as-produced nanoparticles.

Table S1. Summary of Optical Properties for the As-produced SiQDs

Sample	PL Max [nm]	FWHM [nm]	PLQY [%]	τ [μ s]	τ_r [μ s]	k_r [μ s ⁻¹]	τ_{nr} [μ s]	k_{nr} [μ s ⁻¹]	k_r/k_{nr}
N-1	888	163	41.0	251.6	614.5	1.63E-03	426.2	2.35E-03	0.693
N-2	817	183	37.5	199.5	532.5	1.88E-03	319.1	3.13E-03	0.599
N-3	921	137	25.6	N/A	N/A	N/A	N/A	N/A	N/A
N-4	827	220	24.3	184.6	759.2	1.32E-03	243.9	4.10E-03	0.321
Average	864	176	32.1	211.9	635.4	1.61E-03	329.7	3.19E-03	0.538
O-1	926	177	30.1	294.1	976.4	1.02E-03	420.9	2.38E-03	0.431
O-2	809	175	38.2	160.8	420.8	2.38E-03	260.2	3.84E-03	0.618
O-3	827	168	31.7	167.8	529.2	1.89E-03	245.8	4.07E-03	0.464
O-4	841	234	31.3	170.4	544.4	1.84E-03	248.0	4.03E-03	0.455
O-5	946	129	18.8	403.0	2144.4	4.66E-04	496.3	2.01E-03	0.231
Average	870	177	30.0	239.2	923.05	1.52E-03	334.2	3.27E-03	0.440

N = normally-etched SiQDs O = over-etched SiQDs

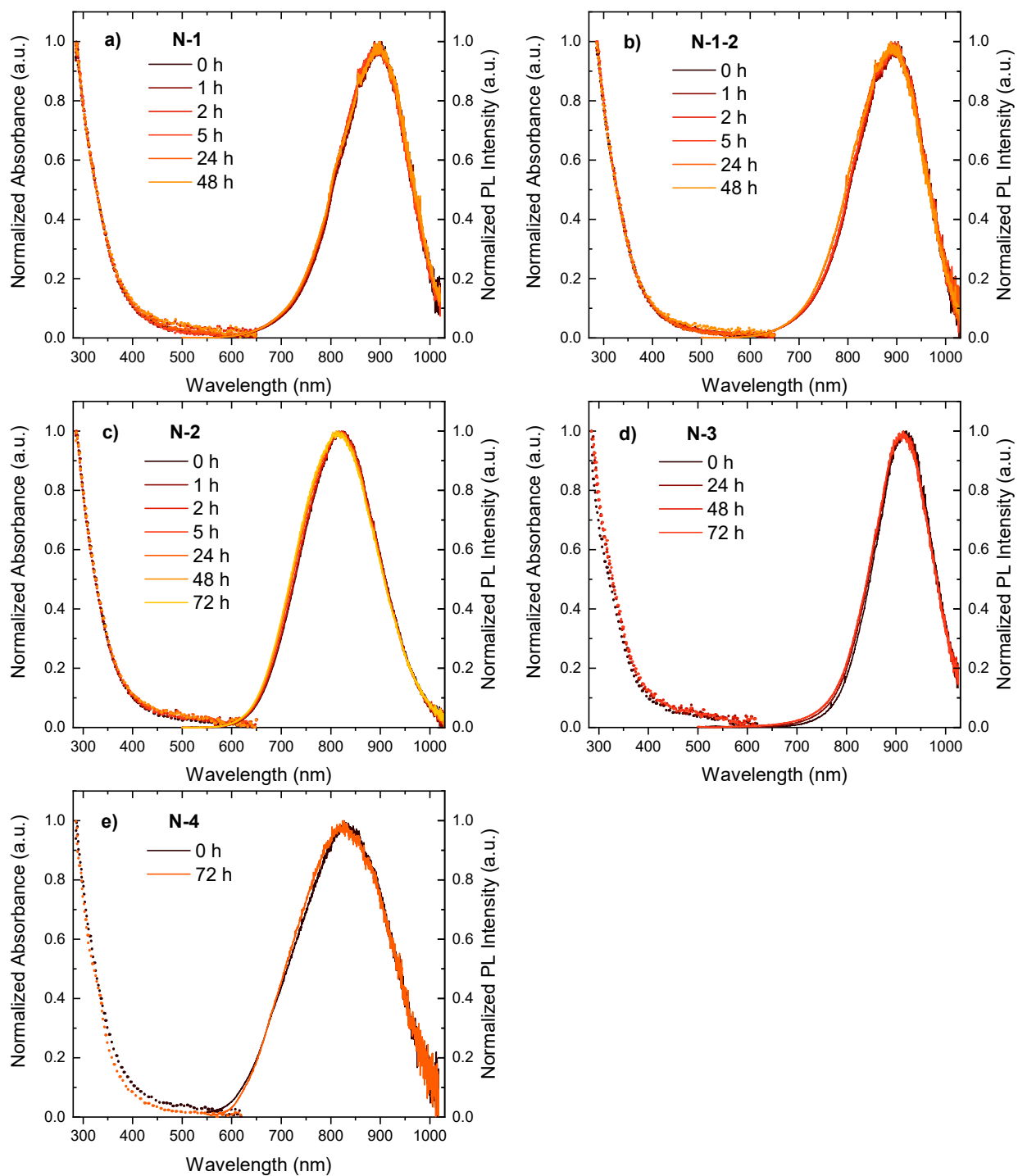


Figure S3. UV-vis absorption (dotted) and PL (solid) spectra of N-SiQDs. The numbering corresponds to Table S1.

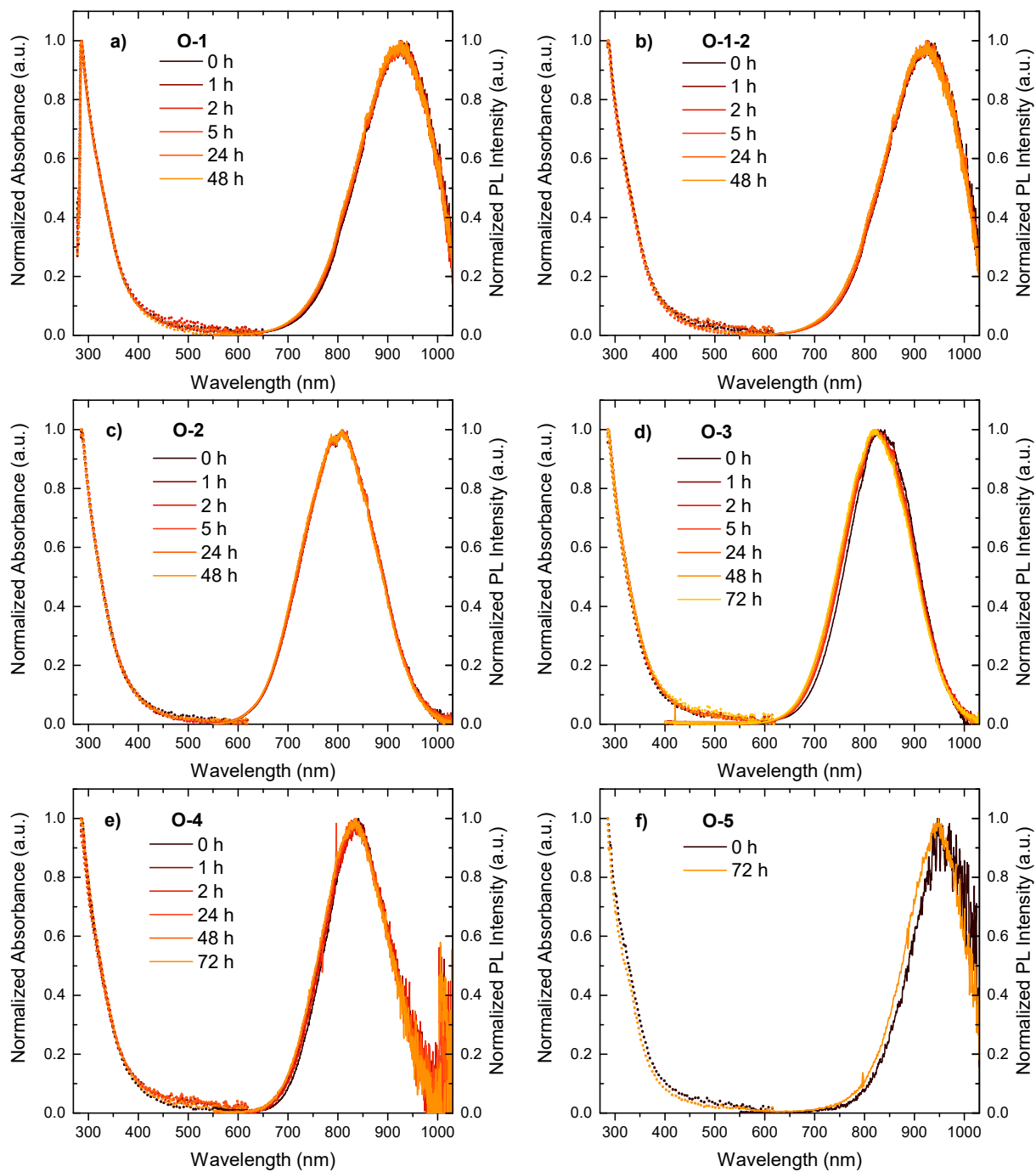


Figure S4. UV-vis absorption (dotted) and PL (solid) spectra of O-SiQDs. The numbering corresponds to Table S1.

Table S2. Summary of Optical Properties for N-SiQDs Throughout Photo-degradation

Sample	Degradation Time [h]	PL Maximum [nm]	FWHM [nm]	PLQY [%]	τ [μ s]	k_r [μ s ⁻¹]	k_{nr} [μ s ⁻¹]	k_r/k_{nr}	Relative Abs @ 365 nm
N-1	0	888	163	41.0	251.6	0.0016	0.0023	0.69	0.22
	1	902	164	41.1	251.1	0.0016	0.0023	0.70	0.22
	2	899	166	39.9	250.6	0.0016	0.0024	0.64	0.23
	5	897	165	37.6	254.7	0.0015	0.0025	0.60	0.22
	24	897	167	36.2	251.1	0.0014	0.0025	0.57	0.23
	48	897	169	28.8	248.4	0.0012	0.0029	0.40	0.24
N-1-2*	0	888	163	41.0	251.6	0.0016	0.0023	0.69	0.22
	1	902	163	41.1	256.2	0.0016	0.0023	0.65	0.21
	2	888	163	39.9	251.6	0.0016	0.0024	0.78	0.23
	5	896	165	37.6	252.7	0.0015	0.0025	0.68	0.22
	24	888	169	36.2	253.2	0.0014	0.0025	0.55	0.22
	48	888	170	27.8	250.1	0.0012	0.0029	0.38	0.23
N-3	0	817	183	37.5	199.5	0.0019	0.0031	0.60	0.22
	1	822	187	31.9	198.0	0.0016	0.0034	0.47	0.22
	2	822	184	43.7	197.6	0.0016	0.0035	0.47	0.23
	5	812	185	30.1	197.4	0.0015	0.0036	0.43	0.22
	24	812	188	29.4	198.0	0.0015	0.0036	0.42	0.22
	48	812	188	29.0	200.9	0.0014	0.0035	0.41	0.23
	72	812	189	26.1	198.3	0.0013	0.0037	0.35	0.23
N-4	0	921	137	25.6	N/A	N/A	N/A	N/A	0.20
	24	915	138	23.0	N/A	N/A	N/A	N/A	0.22
	48	914	141	23.5	N/A	N/A	N/A	N/A	0.22
	72	915	140	21.0	N/A	N/A	N/A	N/A	0.24
N-5	0	827	220	24.3	184.6	0.0013	0.0041	0.32	0.22
	72	824	224	11.5	177.3	0.0006	0.0050	0.13	0.17
Average	0	869	173	33.9	221.9	0.0016	0.0030	0.58	0.22
	1	875	171	38.0	235.1	0.0016	0.0027	0.61	0.22
	2	870	171	41.2	233.3	0.0016	0.0028	0.63	0.23
	5	868	172	35.1	234.9	0.0015	0.0028	0.57	0.22
	24	878	165	31.2	234.1	0.0015	0.0029	0.51	0.22
	48	877	167	27.3	233.2	0.0013	0.0031	0.40	0.23
	72	850	185	19.5	187.8	0.0010	0.0044	0.24	0.21

*N-1-2 is a separate degradation trial using the same SiQDs as N-1.

Table S3. Summary of Optical Properties for O-SiQDs Throughout Photo-degradation

Sample	Degradation Time [h]	PL Maximum [nm]	FWHM [nm]	PLQY [%]	τ [μ s]	k_r [μ s ⁻¹]	k_{nr} [μ s ⁻¹]	k_r/k_{nr}	Relative Abs @ 365 nm
O-1	0	926	177	30.1	294.1	0.0010	0.0024	0.43	0.22
	1	926	182	27.7	299.8	0.0009	0.0024	0.43	0.22
	2	926	177	26.1	297.7	0.0009	0.0024	0.41	0.23
	5	928	179	26.1	304.0	0.0009	0.0023	0.38	0.22
	24	923	181	26.9	304.0	0.0009	0.0024	0.35	0.22
	48	923	184	27.9	303.7	0.0010	0.0022	0.35	0.22
O-1-2*	0	926	177	30.1	294.1	0.0010	0.0024	0.43	0.22
	1	926	178	28.0	298.6	0.0010	0.0023	0.37	0.23
	2	928	178	26.8	302.8	0.0010	0.0024	0.39	0.22
	5	923	178	27.9	307.1	0.0009	0.0024	0.39	0.21
	24	923	180	27.9	303.1	0.0009	0.0024	0.37	0.22
	48	923	180	30.7	308.6	0.0009	0.0024	0.45	0.22
O-3	0	809	175	38.2	160.8	0.0023	0.0039	0.60	0.21
	1	809	176	39.8	159.0	0.0023	0.0040	0.59	0.20
	2	809	178	41.8	159.7	0.0023	0.0039	0.60	0.20
	5	809	175	41.3	157.8	0.0023	0.0041	0.56	0.21
	24	809	175	38.3	158.4	0.0023	0.0040	0.58	0.21
	48	809	178	36.1	154.2	0.0022	0.0043	0.52	0.20
O-4	0	827	168	31.7	167.8	0.0013	0.0060	0.32	0.19
	1	824	162	30.3	164.2	0.0013	0.0061	0.30	0.22
	2	824	162	30.2	163.5	0.0013	0.0061	0.30	0.20
	5	827	162	30.8	164.2	0.0013	0.0061	0.31	0.22
	24	824	164	30.5	163.5	0.0013	0.0061	0.30	0.22
	48	819	165	29.8	161.3	0.0013	0.0062	0.30	0.21
	72	819	164	27.5	161.3	0.0011	0.0062	0.27	0.23
O-5	0	841	234	31.3	170.4	0.0018	0.0040	0.46	0.20
	1	837	169	30.3	175.2	0.0017	0.0040	0.44	0.22
	2	837	209	27.8	167.6	0.0017	0.0043	0.39	0.20
	24	837	209	33.7	178.9	0.0019	0.0037	0.51	0.22
	48	834	195	37.6	192.1	0.0020	0.0033	0.60	0.22
	72	837	236	32.4	186.4	0.0017	0.0036	0.48	0.21
O-6	0	946	129	18.8	403.0	0.0005	0.0020	0.23	0.22
	72	948	135	7.5	402.2	0.0002	0.0023	0.08	0.18
Average	0	870	177	30.0	239.2	0.0014	0.0037	0.41	0.21
	1	864	173	31.2	219.4	0.0014	0.0038	0.42	0.22
	2	865	181	30.6	218.2	0.0014	0.0038	0.42	0.21
	5	872	173	31.5	233.2	0.0013	0.0037	0.41	0.21
	24	863	182	31.5	221.6	0.0014	0.0037	0.42	0.22
	48	862	180	32.4	224.0	0.0015	0.0037	0.45	0.21
	72	868	179	22.5	250.0	0.0010	0.0040	0.28	0.21

*O-1-2 is a separate degradation trial using the same SiQDs as O-1.

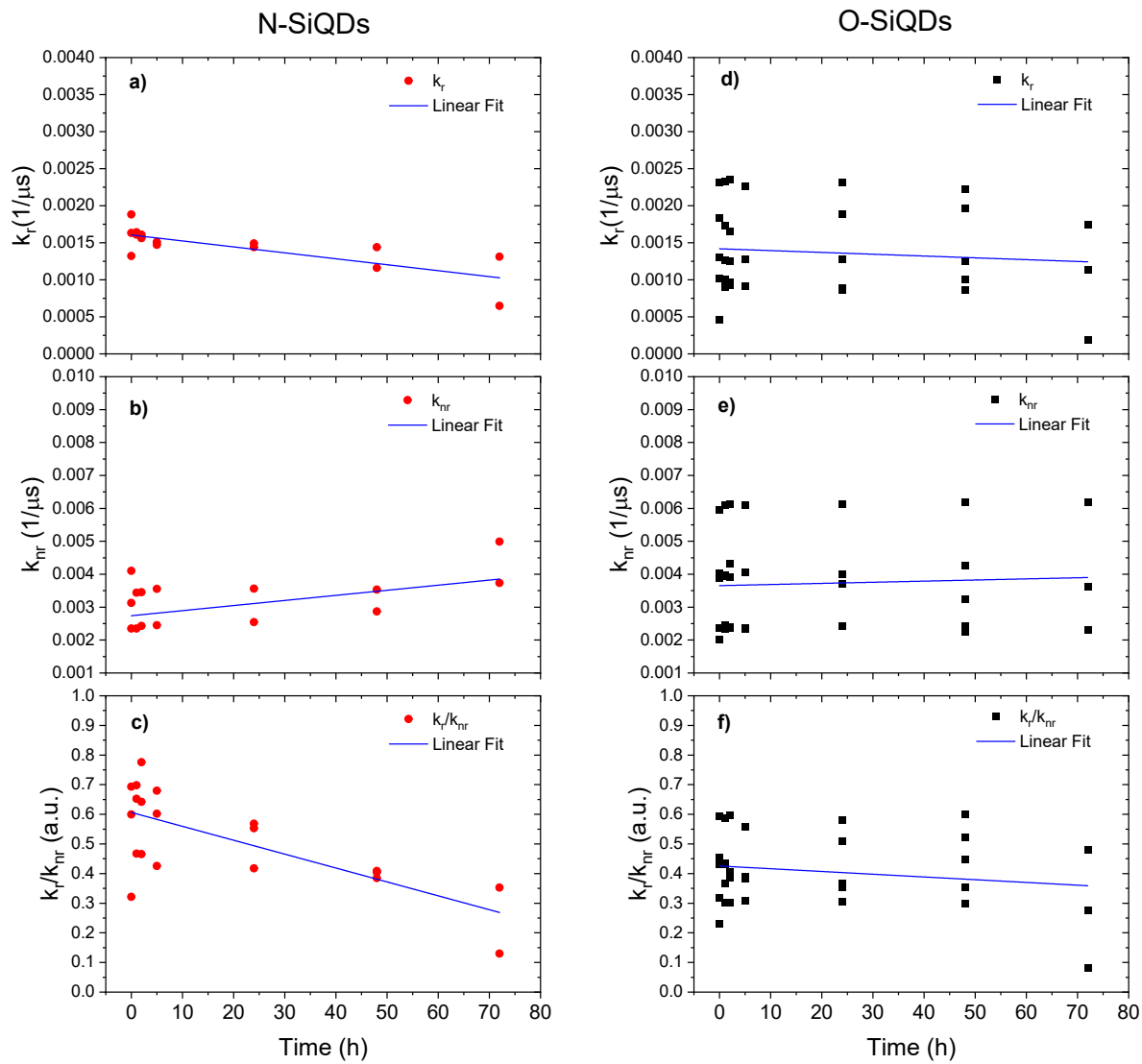


Figure S5. Linear fit of k_r , k_{nr} , and k_r/k_{nr} of SiQDs (a-c for N-SiQDs and c-d for O-SiQDs).

Table S4. Summary of Linear Fit for SiQDs Recombination Rate

Sample			Value	Standard Error	t-value	P-value
N-SiQDs	k_r	Intercept	0.0016	4.32375E-5	37.11502	0
		Slope	-8.02471E-6	1.43376E-6	-5.59697	2.13358E-5
	k_{nr}	Intercept	0.00274	1.72603E-4	15.86944	2.03459E-12
		Slope	1.54649E-5	5.72354E-6	2.70198	0.01413
	k_r/k_{nr}	Intercept	0.60632	0.03175	19.09527	7.37188E-14
		Slope	-0.00469	0.00105	-4.45414	2.72092E-4
O-SiQDs	k_r	Intercept	0.00142	1.308E-4	10.84687	4.44089E-12
		Slope	-2.4474E-6	4.33258E-6	-0.56488	0.57622
	k_{nr}	Intercept	0.00365	3.25774E-4	11.21471	1.93623E-12
		Slope	3.41376E-6	1.07909E-5	0.31636	0.75385
	k_r/k_{nr}	Intercept	0.4256	0.02634	16.16049	2.22045E-16
		Slope	-9.2474E-4	8.72351E-4	-1.06005	0.29731

The t-value is a measure of how many standard errors the estimated value is away from zero (i.e, slope = zero). A higher absolute t-value suggests that the estimate is more likely to be reliable. The P-value indicates the likelihood of the null hypothesis (i.e., there is no relationship between the independent variable and the dependent variable). A low p-value (typically < 0.05) suggests that one can reject the null hypothesis.

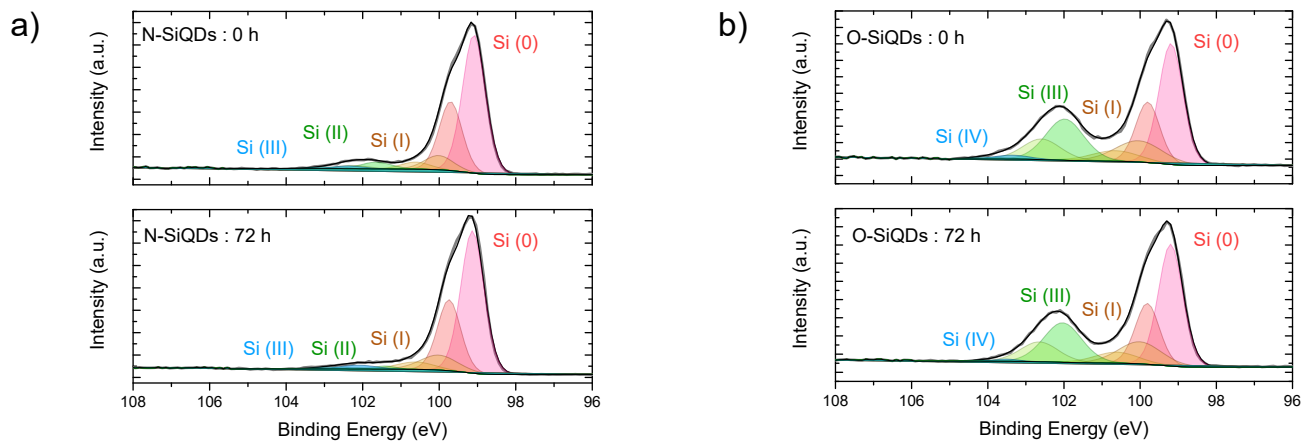


Figure S6. High-resolution Si 2p XP spectra of a) N-SiQDs and b) O-SiQDs with (top) and without (bottom) 72 h of UV irradiation.

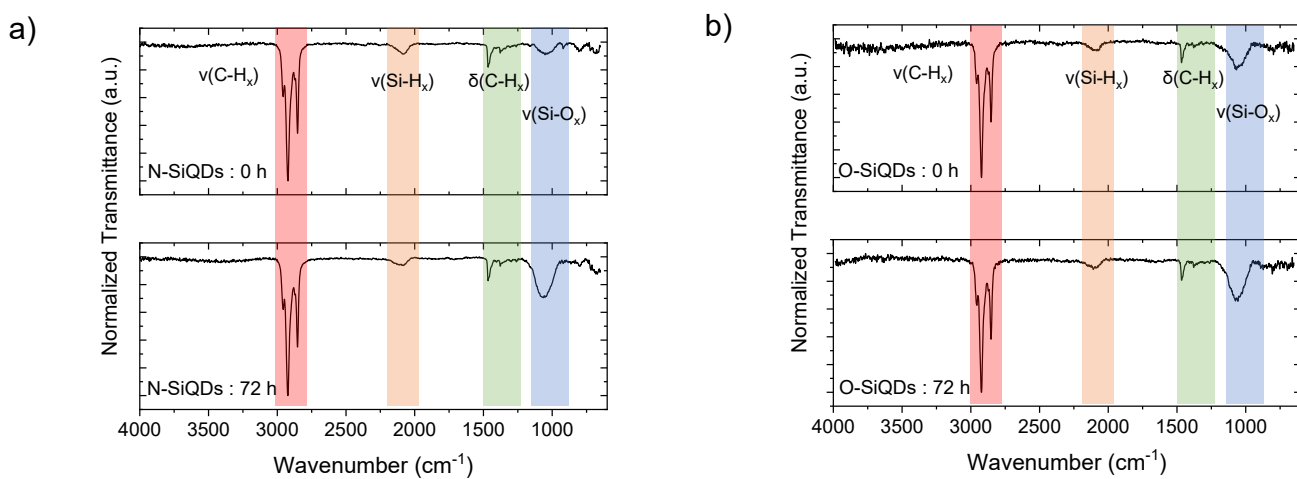


Figure S7. FT-IR of a) N-SiQDs and b) O-SiQDs with (top) and without (bottom) 72 h of UV irradiation.

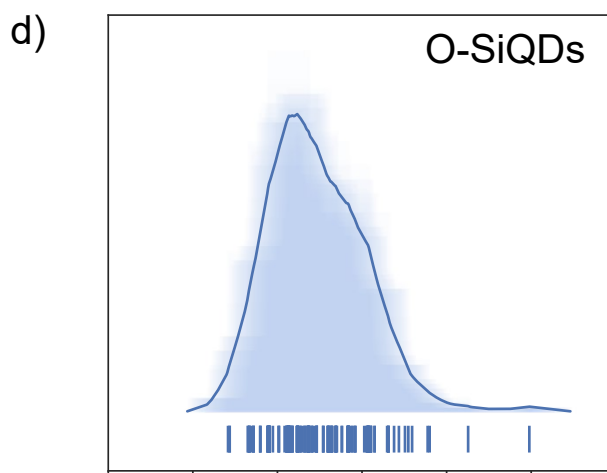
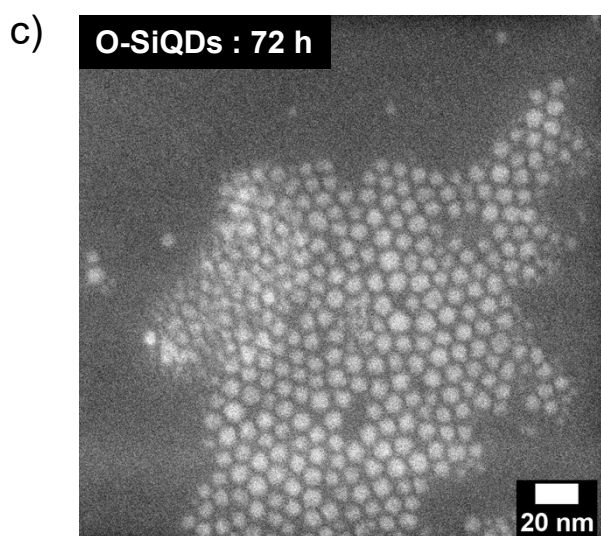
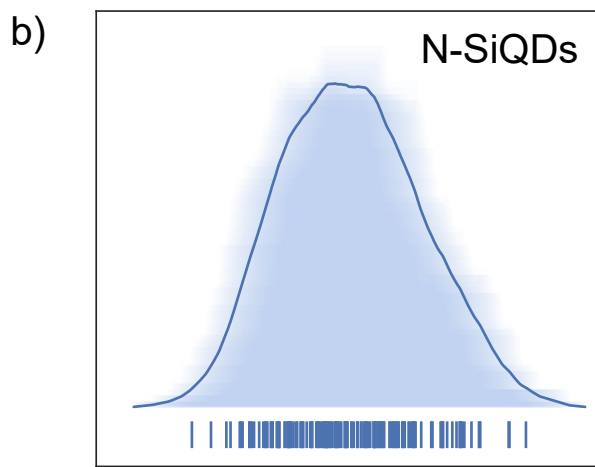
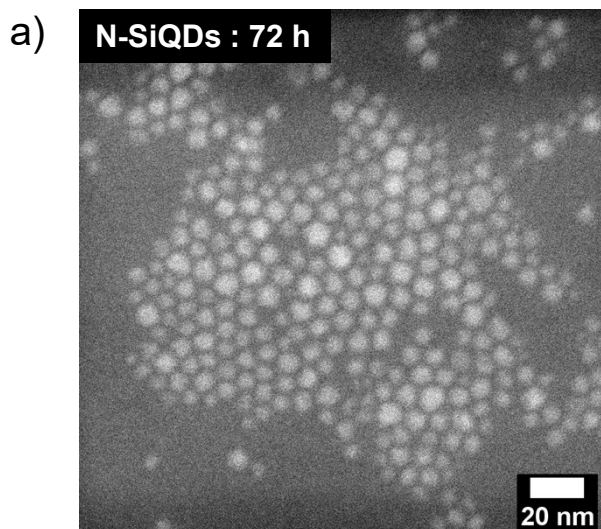


Figure S8. Dark-field TEM images of a) N-SiQDs and c) O-SiQDs) after 72 h of UV exposure. Average-shifted histogram showing the size distribution of the degraded b) N-SiQDs and d) O-SiQDs from corresponding TEM images.