Supporting Information

Optical extinction spectra of silicon nanocrystals: Size dependence on the lowest direct transition

Ryan Gresback¹, Yoichi Murakami², Yi Ding¹, Riku Yamada¹, Ken Okazaki¹, Tomohiro Nozaki^{1*}

 Department of Mechanical and Control Engineering, Graduate School of Science and Engineering, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku, Tokyo 152-8552, Japan

2. Global Edge Institute, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro-ku,

Tokyo 152-8550, Japan

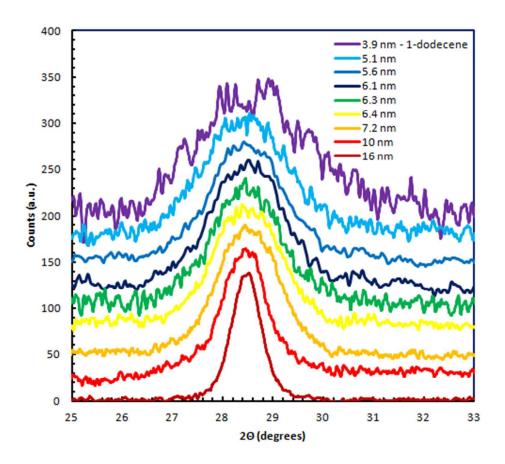


Figure S1. XRD pattern of Si NC (111) reflection for described in Figure 1.

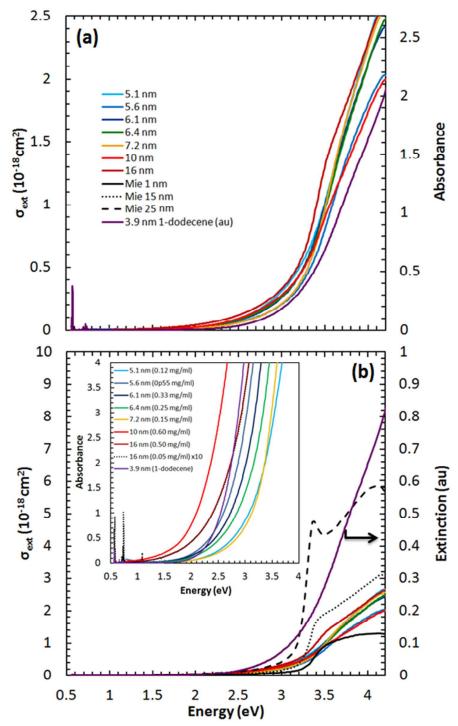


Figure S2. (a) Per-atom extinction spectra (left axis) and raw absorbance (right axis) on linear-scale of colloidal Si NCs in benzonitrile with concentrations of 0.05 mg/ml (colored traces) and 1-dodecene treated Si NCs with unknown concentration in toluene (purple). NC sizes in legend determined by XRD and (b) rescaled and compared with (black traces) the Mie solution. Inset: High concentration extinction spectra with raw absorbance values and (dotted) 16 nm Si NCs with concentration of 0.05 mg/ml scaled by a factor of 10 showing linearity at high absorbance values and scaling according to Beer's law.

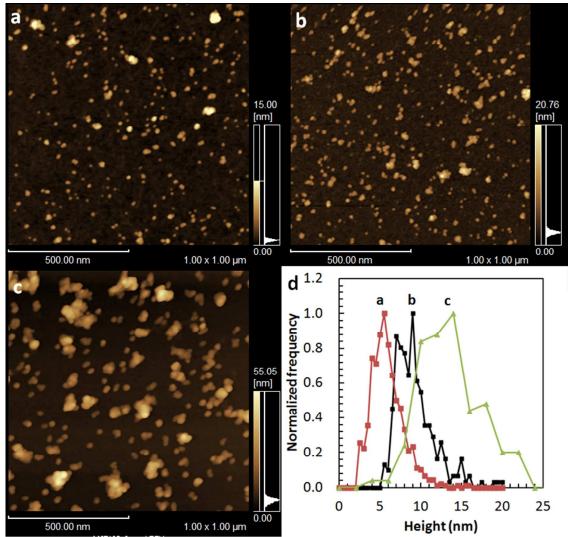


Figure S3. AFM height traces of Si NCs mean XRD sizes of: a) 5.1 nm, b) 7.2 nm and c) 10 nm spin cast from benzonitrile onto polished silicon substrates and d) distribution of maximum NC height where the mean and standard deviations are 5.4 ± 1.6 nm, 8.5 ± 2.0 nm, and 13.2 ± 3.7 nm for a, b and c, respectively.

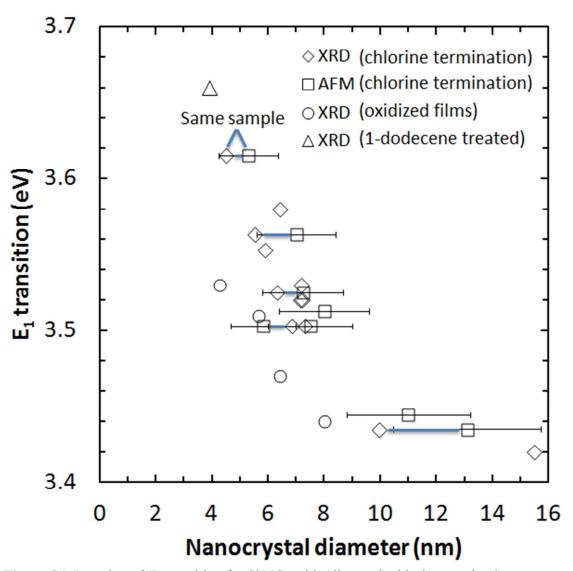
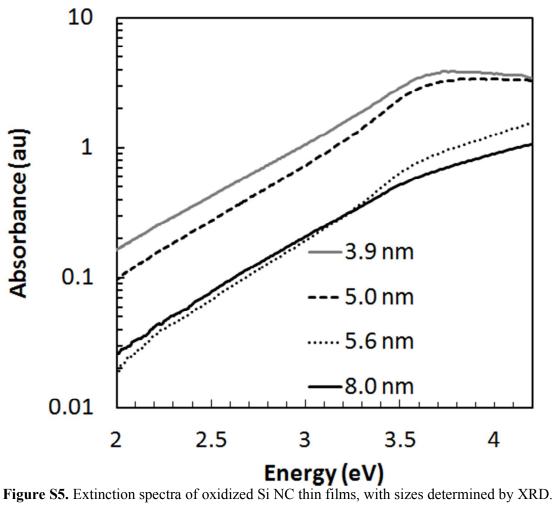
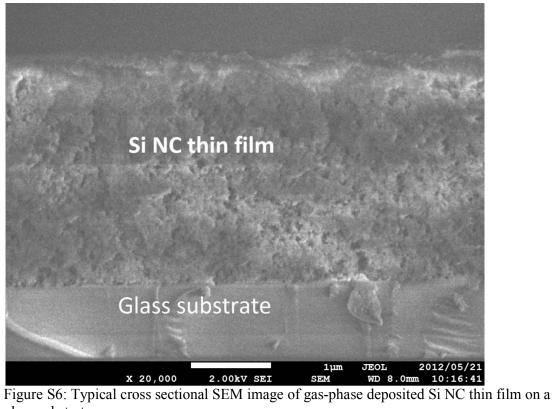


Figure S4. Location of E_1 transition for Si NCs with (diamond) chlorine termination, (triangle) 1-dodecene treated, and (circle) oxidized film with sizes determined by XRD, and size and distribution from (square) AFM. Horizontal blue line connecting XRD and AFM points indicates the samples were fabricated from the same colloid.





glass substrate.

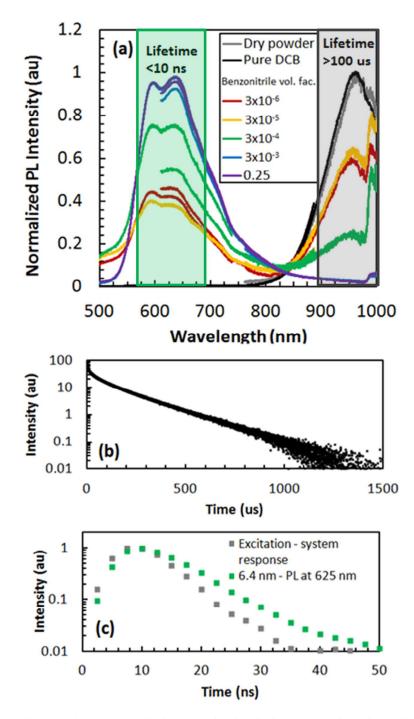


Figure S7: (a) Photoluminescence of SiCl₄ synthesized Si NCs as a function of environment for (grey) as produced as-free powder (black) in 1,2-dichlorobenzene (DCB) and (colored) in DCB with different volume fractions of benzonitrile and PL decay of Si NCs in (b) DCB only with a PL lifetime of ~180 μ s and (c) benzonitrile with a lifetime of < 10 ns (green) and system response (grey).

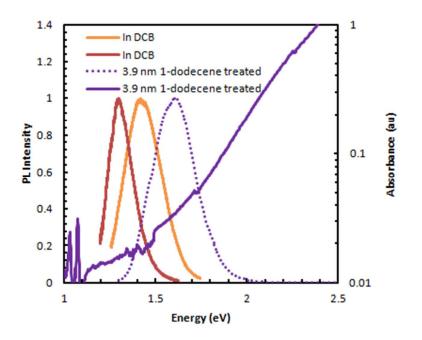


Figure S8: Photoluminescence of Si NCs in (red and orange) in DCB and (purple dash) 1-dodecene treated Si NCs in toluene and (purple solid) absorbance of 1-dodecene treated Si NCs in toluene (\sim 220 µs PL lifetime).