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Effects of oxidation on the photoluminescence from silicon nanoparticles.

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Understanding the stability of silicon nanoparticles (Si-np) in oxidative environments is important to their use as a luminescent marker in biophysical applications. Treatments with NaOH, HCl, and UV radiation lead to substantial red-shifts in the emission from ultrasmall (~1.0 nm) Si-np. Modeling of the photoluminescence (PL) spectra shows the same set of three distinct, narrow (~0.47 eV), near-Gaussian emissions with their relative strengths varying among the treatments. From the expected chemical and structural effects of the treatments and the results of computational modeling, each distinct emission is correlated with its probable chemical origin. A simple model of surface oxidation captures the general behavior and PL properties of this system. These results offer the exciting possibility of tailoring the PL properties of Si-np through control of their surface chemistry. Supported by the NIH, PHS 5 P41-RRO3155, and by UIUC.