Revisiting an Ongoing Debate: What Role do Surface Groups Play in Silicon Nanocrystal Photoluminescence?

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Tailorable surface chemistry and tunable optical response of Silicon nanocrystals (Si NCs) make them appealing active materials for optoelectronic applications. However, the origin of photoluminescence (PL) of silicon nanocrystals (SiNCs) remains a subject of considerable debate. Size-dependant PL that supports the quantum confinement model has been proposed by several researchers. [1,2] On the other hand, SiNC PL arising from surface states that are independent of nanocrystal size has also been shown. [3]

This work addresses the origin of surface-functionalized SiNC PL as relating to surface states and the NC size. SiNCs of different sizes (3 and 5 nm diameters) were prepared with three distinct surface chemistries. Steady state and time-resolved PL measurements were performed at temperatures ranging from 37 to 377 K. The role of oxygen on SiNC PL was further investigated by controlled oxidation of size-selected SiNCs. Insights gained from this study are used to propose a general emission mechanism for the observed phenomena.

1) A. Hartel *et al*., *Phys. Rev. B* **2012***, 85*, 165306.
2) F. Maier-Flaig *et al*., *Chem. Phys.* **2012***, 405*, 175.
3) M. Dasog *et al*., *Nano* **2014***, 8*, 9636.