Supplementary Materials

Microscopic Proof of Photoluminescence from Mechanochemically Synthesized 1-Octene Capped Quantum Confined Silicon Nanoparticles: Implications for Light Emission Applications

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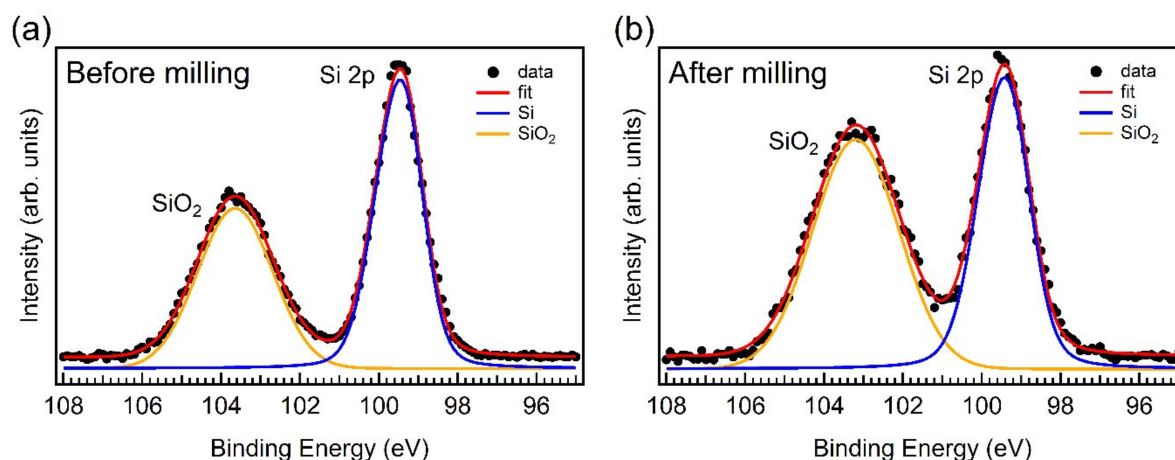
1. XPS Measurements:

In both spectra, the Si 2p region is characterized by two peaks, ascribed to elemental Si and SiO_2. Our reference sample, i.e. the Si microparticles before the milling, displays the main elemental Si peak at 99.4 eV of binding energy and the broader SiO_2 peak at 103.6 eV, in good agreement with literature[1]. From the peak areas obtained from the fit (red curve), we obtain a $SiO_2/(Si+SiO_2)$ ratio of 0.45. The presence of the oxide species suggests that the Si microparticles are oxide capped. Similarly, the milled silicon particles display the main elemental Si peak at 99.3 eV of binding energy and the SiO_2 peak at 103.2 eV. The $SiO_2/(Si+SiO_2)$ ratio increased to 0.55, indicating not only an oxide capping but also an increase of the total oxide species compared to elemental Si. However, the high surface sensitivity of XPS is expected to enhance the signal from an oxide capping layer, which is why these results are not representative for the SiO_2 content of the entire Si nanoparticle.



(c)

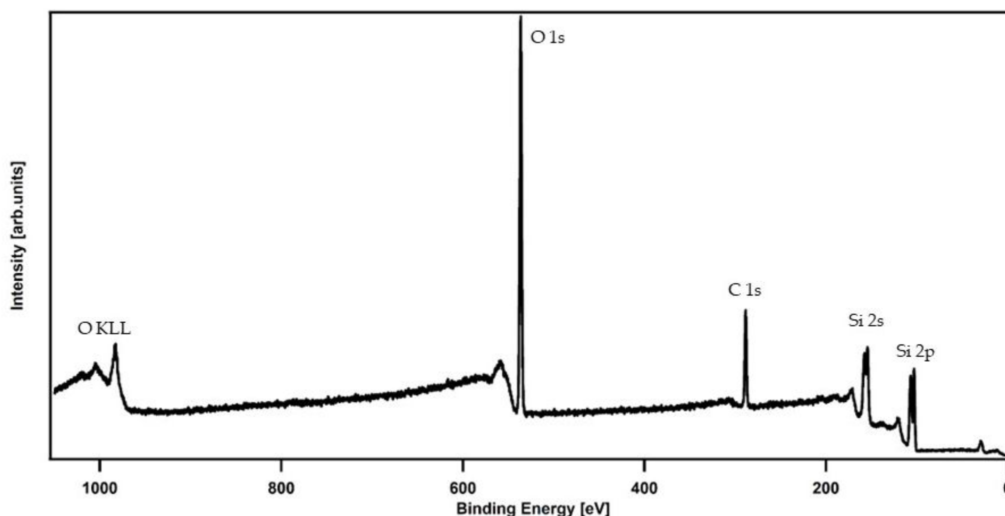


Figure S1: XPS measurements of the silicon particles Si 2p region before (a) and after the milling (b). The data points are depicted as black dots and the resulting fit as a red curve. The corresponding peaks ascribed to elemental Si and SiO_2 are depicted with a blue and an orange curve, respectively. The Si nanoparticles are oxide capped and the relative intensity of SiO_2 increases after milling. (c) XPS survey spectrum. The spectrum has been taken at the highest pass energy (500 eV) with a long integration time: only oxygen, carbon and silicon are present, with no traces of impurities.

2. **XRD Measurements:**

XRD of milled and un-milled silicon particles shows no changes in phase, which remained diamond cubic after milling and passivation (Fig. S2). In the milled sample, we observe broadening of the peaks and a low intensity SiC peak[2] which suggest that milling reduced the particle size, increased the strains, while passivation with carbon ligands caused some reaction between Si and C leading to SiC formation.

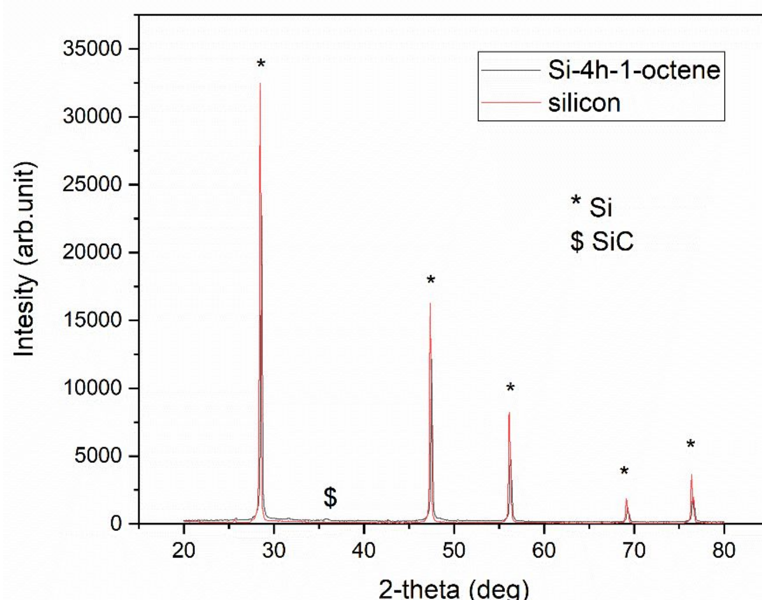


Figure S2: X-ray diffraction patterns of the un-milled (in Red) and milled Si (in Black) particles. Both the spectrum are overlapping on each other without change in peak positions, suggest no change in the phase of Si particles after milling. A small-intensity SiC peak is present in the milled sample that is expected due to reaction between Si and 1-octene.

3. **DLS Measurements:**

DLS is performed to study the particle size distribution (Fig. S3) in the milled powders before the size separation. The results suggest a broad size distribution from 100 nm to 1000 nm sized particles in the sample. However, the size distribution did not reveal particles below 10 nm in size. This could be due to a low concentration of such particles.

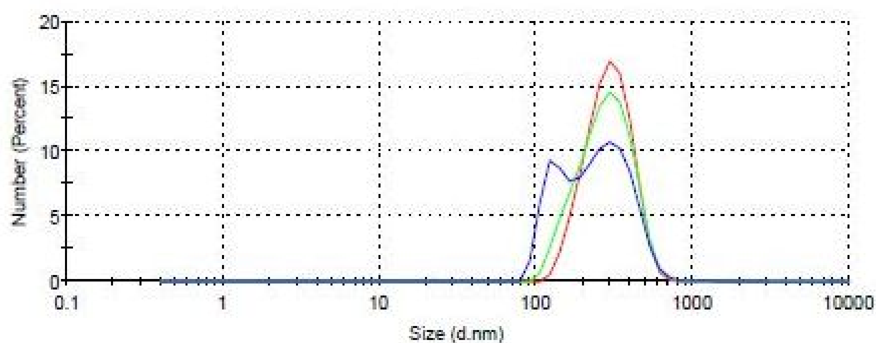


Figure S3: Dynamic light scattering results of milled Si nanocrystals showing particle size distribution of 100-1000 nm in the sample before size separation. The weighted average of the particle sizes is 330 nm with 97 % std. dev.

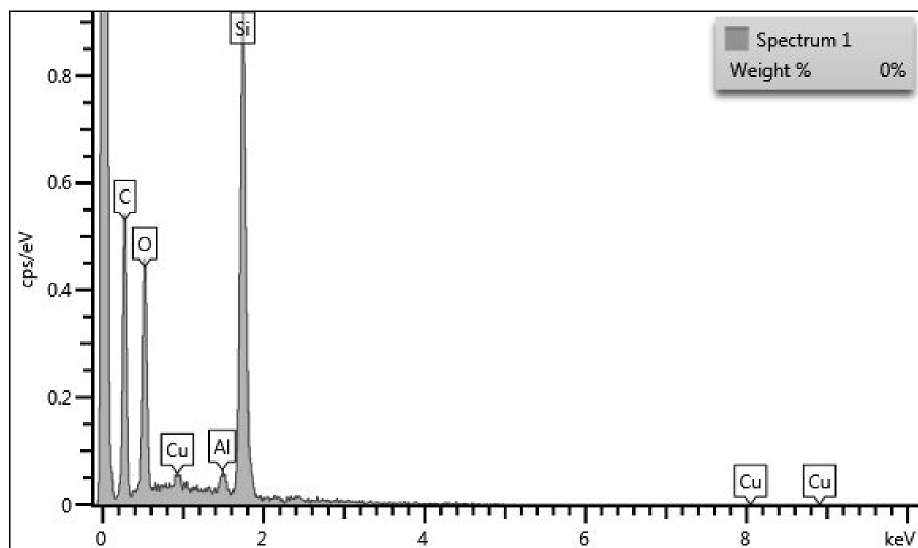


Figure S4: EDX spectrum of the milled Si nanocrystals drop cased on the carbon coated copper grid.

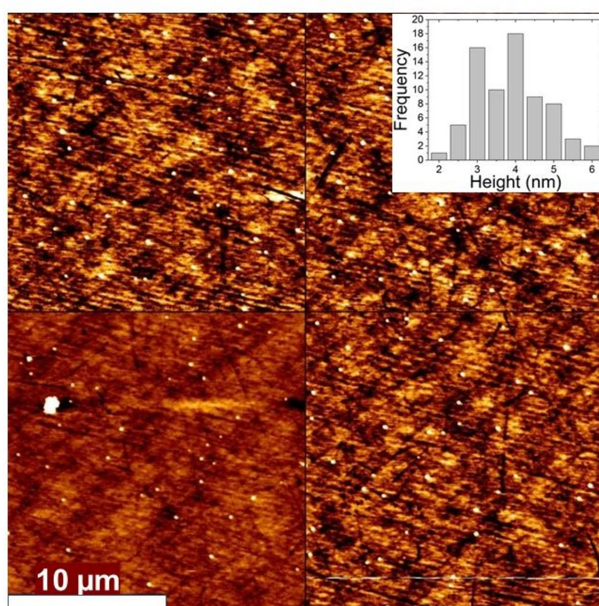


Figure S5: AFM image of 1-octene capped SiNCs. Inset is showing a histogram of particle size distribution in the AFM image. Particles of sizes 2-6 nm are present in the sample.

References:

1. Naumkin, A.V.; Kraut-Vass, A.; Gaarenstroom, S. W.; Powell, C.J. NIST X-ray Photoelectron Spectroscopy Database, NIST Standard Reference Database 20, Version 4.1 (Web version) (doi: 10.18434/T4T88K) **2012**.
2. Iwanowski, R. J; Fronc, K.; Paszkowicz, W.; Heinonen, M. XPS and XRD study of crystalline 3C-SiC grown by sublimation method, *Journal of Alloys and Compounds*, **1999**, 286, 143-147.