Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Electronic Supplementary Information

A Novel Sustainable and Green Mechanochemical Route from $(HSiO_{1.5})_n$ Polymer to Emissive Silicon Nanocrystals

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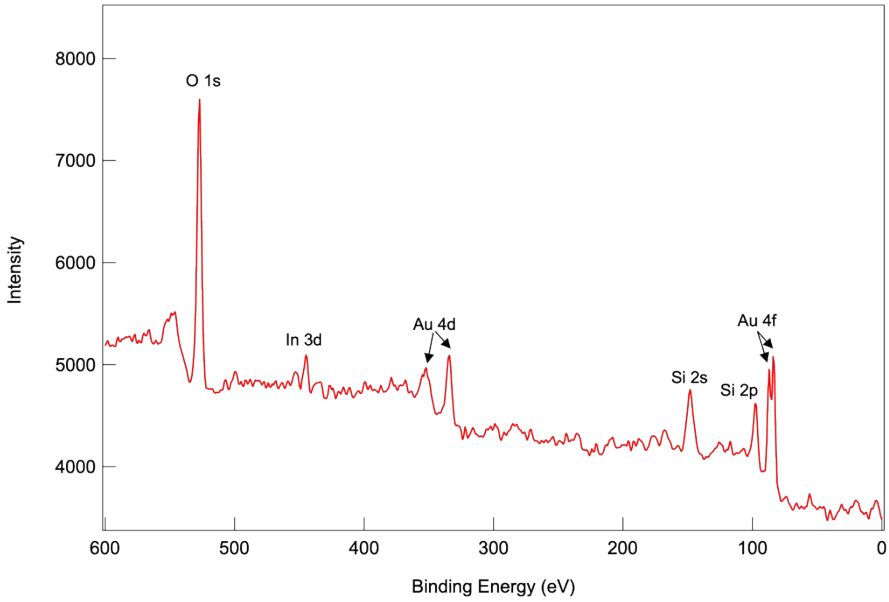

Figure S1. XPS survey spectra of the mechanochemically treated $(HSiO_{1.5})_n$ polymer with milling balls in size of 10 mm at a rotation speed of 400 rpm in 3 hours (B10_T3h). In 3d comes from substrate of measurement, and Au is used for calibration. Si 2p, Si 2s and O 1s are attributed to pure $(HSiO_{1.5})_n$ polymer without Zr-related impurities after the mechanochemical process.

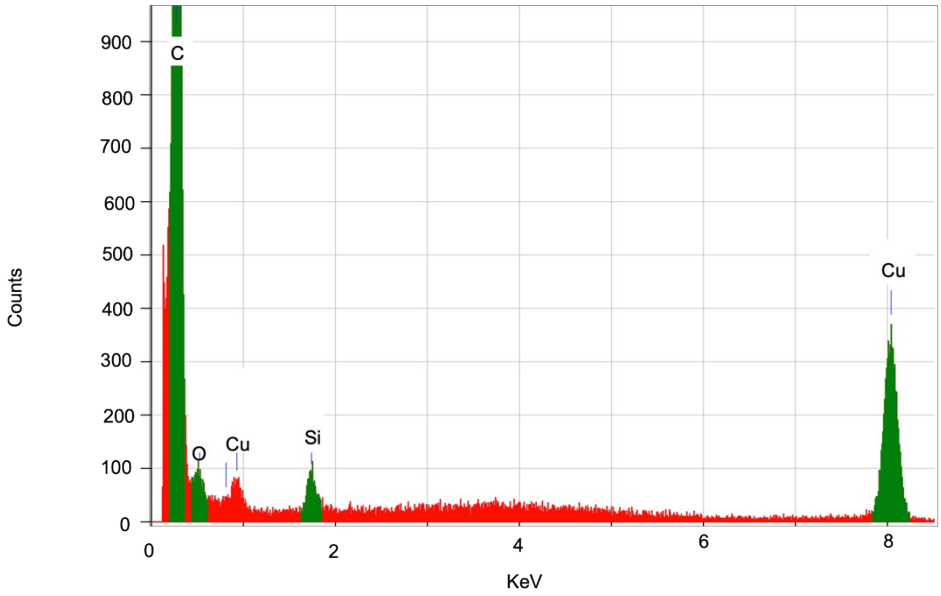

Figure S2. EDX spectra of mechanochemically treated $(HSiO_{1.5})_n$ polymer with milling balls in size of 10 mm at a rotation speed of 400 rpm in 3 hours (B10_T3h). C, Cu are collected from the grid for measurement. Peaks of Si and O exemplifies the presence of Si and O components, without Zr-related impurities after the mechanochemical process.

In terms of sustainability, We calculated the electric energy consumptions of a lab-made tube furnace and a high-energy planetary ball-mill (Fritsch, Pulverisette 7) equipment for processing the same amount of $(HSiO_{1.5})_n$ polymer towards synthesis of Si NCs via thermal- or mechanochemical approaches, respectively. Specifically, the $(HSiO_{1.5})_n$ polymer was pyrolyzed under flowing 95% Ar/ 5% H_2 with a flux rate of 250 mL/min from room temperature to 1100 °C for 2.5 h, and held at 1100 °C for 1 h, then cooling to room temperature naturally. Under the condition of mechanochemical route, $(HSiO_{1.5})_n$ polymer were processed for 3 h in a sealed milling vessel (80 mL, filling rate: 10%) fulfilled with Ar. The electric energy consumption W is calculated by

$$W = PT$$

where P is the power consumption of devices which was measured by a clamp power logger (ZN-CTC11, OMRON Corp.) for a tube furnace or recorded by the EASY GTM-System equipped in a milling vessel. The monitored results are shown as Fig. S3. T is the electric supply time, which is equal to at least 3.5 h (2.5 h for heating process, in addition, holding at 1100 for 1 h) and 3 h for mechanochemical process.

As a result, in the case of thermal pyrolysis, W = 2.359 kW · h = 8.492 x 10^6 J, while for mechanochemically treatment process, W = 0.162 kW · h = 5.843 x 10^5 J. Therefore, the energy consumption of thermal pyrolysis is almost 15 times higher than planetary ball milling process.

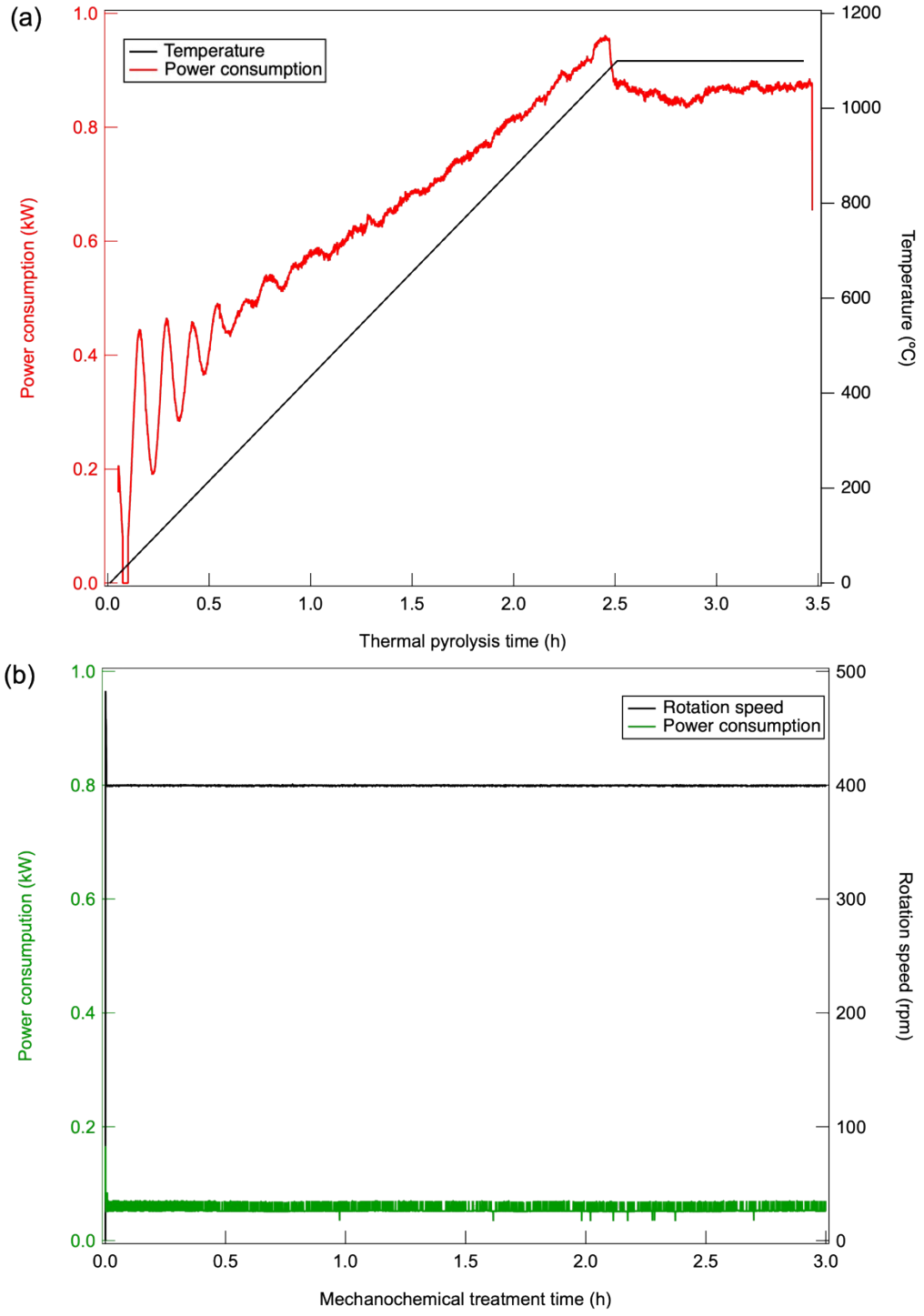

Figure S3. (a) Power consumption of a tube furnace for synthesis of Si NCs via high temperature thermal pyrolysis of $(HSiO_{1.5})_n$ polymer (b) power consumption of a high-energy planetary ball-mill equipment for processing the same amount of $(HSiO_{1.5})_n$ polymer towards synthesis of Si NCs via mechanochemically treatment process.

Table S1. Comparison between conventional high temperature induced thermal pyrolysis and the proposed mechanochemical route of $(HSiO_{1.5})_n$ polymer for emissive free-standing Si NCs synthesis and their optical properties.

Synthesis route	Conditions	Surface passivation	Size/nm	PL wavelength/nm	QY	Ref.
Thermal pyrolysis	1100 °C, 1 h 5% H_2/95% Ar	Decyl-	3.2	600~650	NA	*1*
Thermal pyrolysis	1100 °C, 1 h, 5% H_2/95% Ar	Dodecyl-	1.2	420	3%	*2*
Thermal pyrolysis	1100 °C, 1 h, 5% H_2/95% Ar	allylbenzene-	1.0	600	5%	*3*
Thermal pyrolysis	1100 °C, 1 h 5% H_2/95% Ar	Dodecyl-	4.6	800	10%	*4*
Mechanochemical route	10 mm, 400 rpm, 3 h	Decyl-	4.8	610	9.8%	***This work***

References

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