Electronic Supplementary Information

Synthesis by Size Focusing of Lithium Tantalate Nanoparticles with a Tunable Second Harmonic Optical Activity

Rana Faryad Ali[†], *Byron D. Gates*[*,†]

[†] Department of Chemistry and 4D LABS, Simon Fraser University, 8888 University Drive, Burnaby, BC, V5A 1S6, Canada

[*] E-mail: bgates@sfu.ca

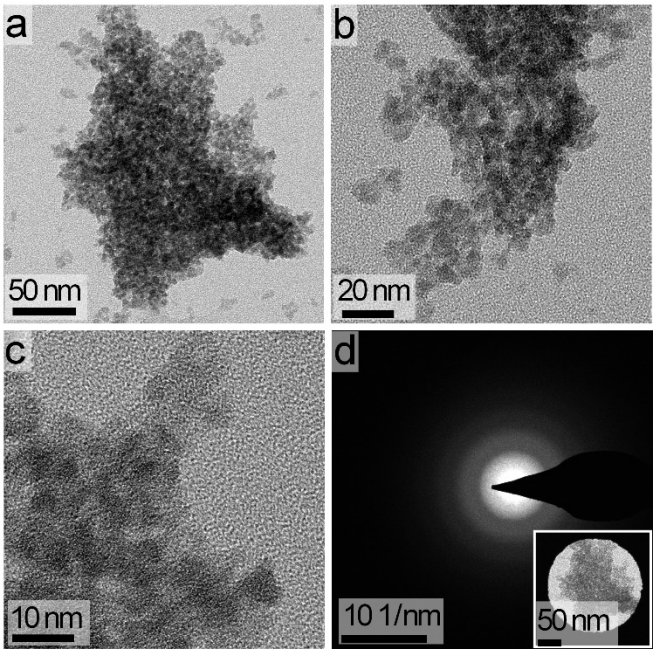

Figure S1. The product obtained after 3 d of solvothermal treatment of the precursors as characterized by: (a, b) transmission electron microscopy (TEM); (c) a high-resolution (HR) TEM (or HRTEM) analysis; and (d) a selected area electron diffraction (SAED) based analysis.

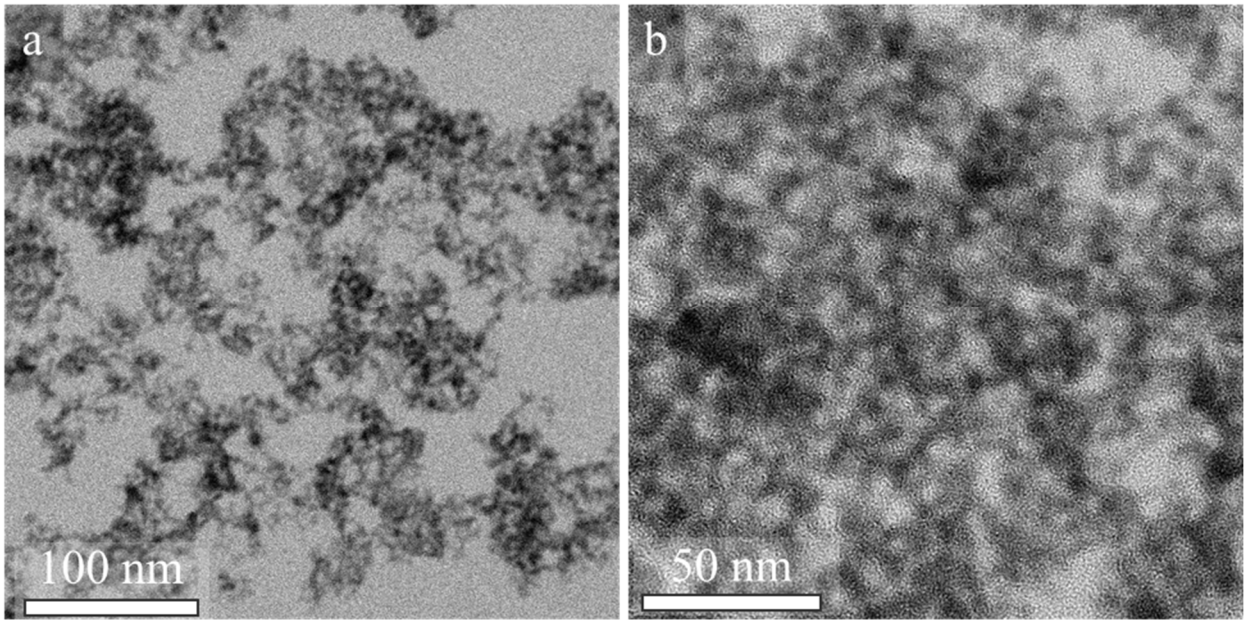

Figure S2. A HRTEM analysis of lithium tantalate ($LiTaO_3$) nanoparticles (NPs) obtained after a solvothermal treatment for 4 d, which indicates the formation of relatively small particles.

Table S1. Ratios the peak areas as measured by X-ray diffraction (XRD) relative to the (012) reflection for the reported $LiTaO_3$ reference material (ICSD No. 9537) and for NPs of $LiTaO_3$ prepared between reaction times of 4 d and 7 d.

XRD peak ratios	Reference ICSD No. 9537	4 d product	5 d product	6 d product	7 d product
(104)/(012)	0.40	0.73	0.79	0.74	0.56
(110)/(012)	0.29	0.71	0.76	0.72	0.51
(202)/(012)	0.14	0.39	0.65	0.61	0.44
(024)/(012)	0.18	0.50	1.55	0.63	0.46
(116)/(012)	0.26	0.61	1.03	0.75	0.52
(214)/(012)	0.15	0.48	0.78	0.62	0.45

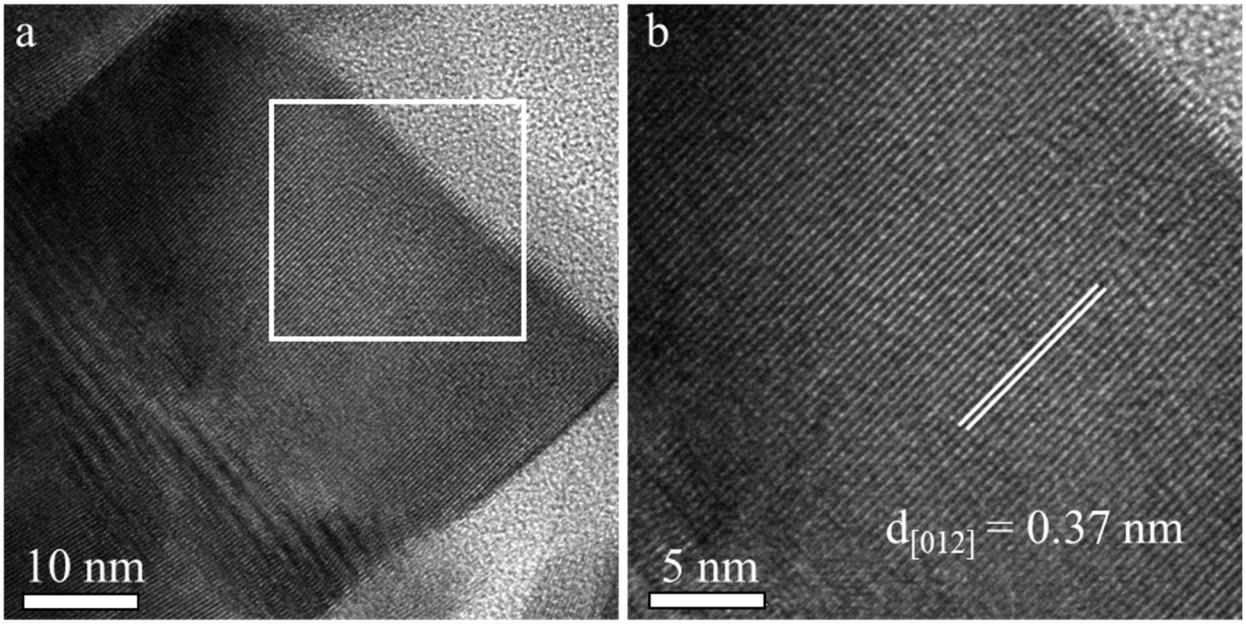

Figure S3. (a) Representative results from a HRTEM analysis of the $LiTaO_3$ NPs obtained at a solvothermal reaction time of 5 d. (b) A higher magnification of the sample obtained from the region indicated by the white box in (a). The white lines highlight the observed lattice fringe patterns, whose d-spacing is assigned on the image.

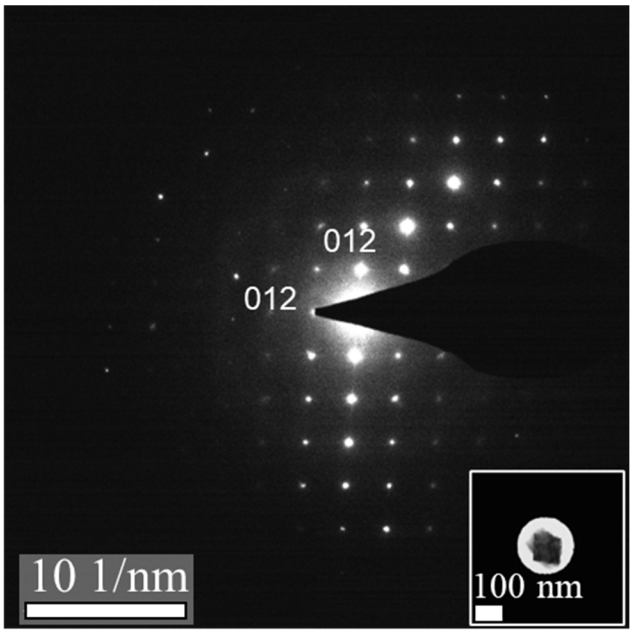

Figure S4. The selected area electron diffraction (SAED) pattern obtained from a single NP (shown within the inset). The SAED pattern indicates the crystalline nature of this $LiTaO_3$ NP, which was obtained after 5 d of solvothermal treatment.

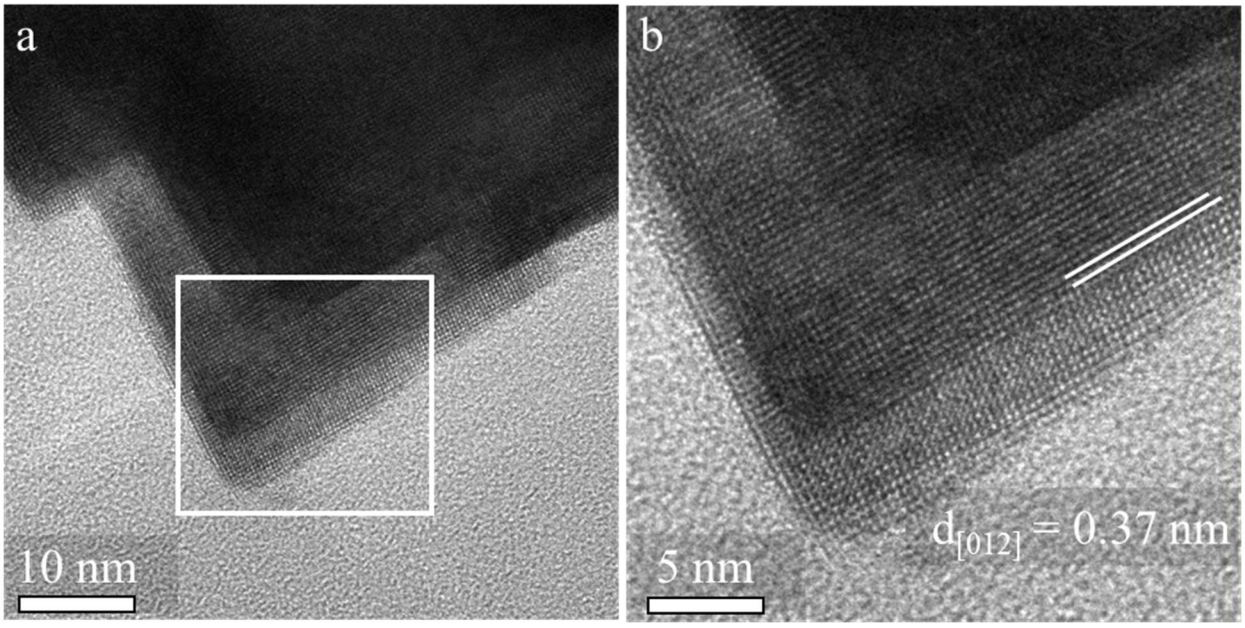

Figure S5. (a) Representative results from a HRTEM analysis of $LiTaO_3$ NPs obtained after a reaction time of 6 d. (b) A higher magnification of the sample obtained from the region indicated by the white box in (a). The white lines highlight the observed fringe patterns, whose d-spacing is assigned on the image.

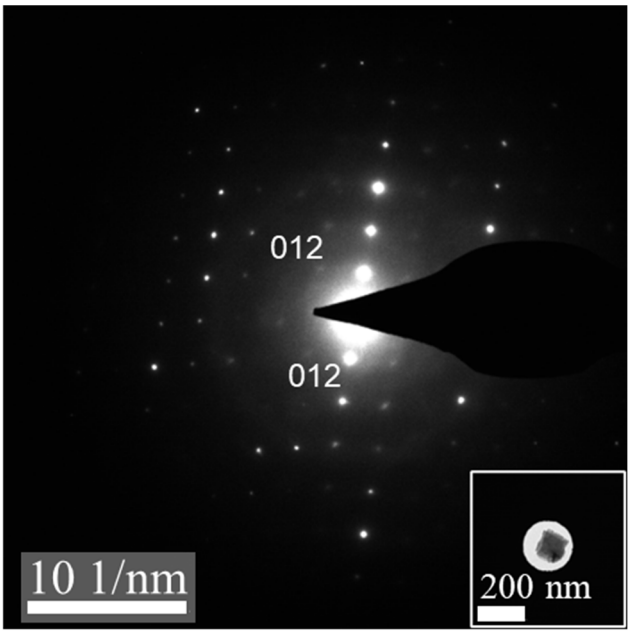

Figure S6. The selected area electron diffraction (SAED) from a single NP (shown within the inset). The SAED pattern indicates the crystalline nature of the $LiTaO_3$ NPs obtained after a reaction time of 6 d as discussed in further detail in the main text.

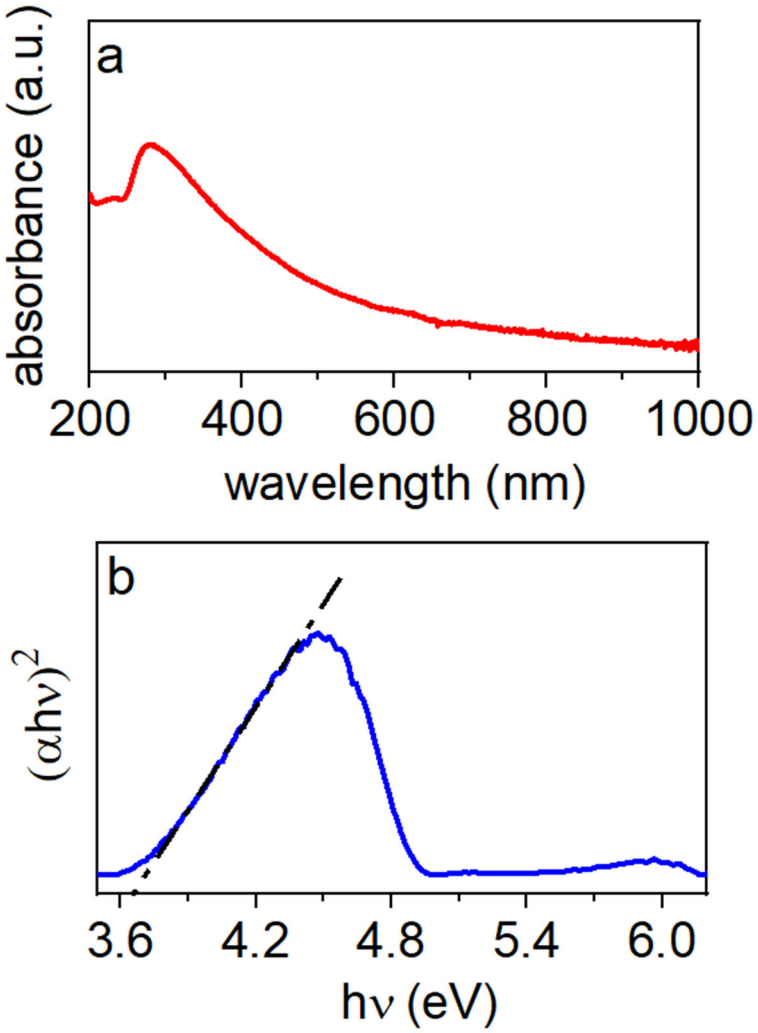

Figure S7: (a) Ultraviolet (UV)-visible absorbance spectrum for a suspension of $LiTaO_3$ nanoparticles in ethanol. This spectrum indicates the optical transparency of these nanoparticles from >350 nm to 1,000 nm. (b) Analysis of the optical bandgap for the $LiTaO_3$ nanoparticles as determined using a Tauc plot. The Tauc plot was obtained by plotting $(\alpha h\nu)^{1/n}$ versus the incident light in values of hν, where α represents the absorption coefficient and n denotes the type of electronic transition involved in the excitation process. A value of n = 2 was used for these analyses, which corresponds to an indirect bandgap transition. The calculated bandgap is 3.64 eV or ~340 nm, which is consistent with prior reports for $LiTaO_3$.[1,2]

References

(1) Ismangil, A.; Jenie, R. P. Development of Lithium Tantallite ($LiTaO_3$) for Automatic Switch on LAPAN-IPB Satellite Infra-Red Sensor. *Procedia Environmental Sciences* **2015**, *24*, 329–334.

(2) Wang, C.; Li, Z.; Riemensberger, J.; Lihachev, G.; Churaev, M.; Kao, W.; Ji, X.; Zhang, J.; Blesin, T.; Davydova, A. Lithium Tantalate Photonic Integrated Circuits for Volume Manufacturing. *Nature* **2024**, 1–7.