Electronic Supplementary Material (ESI) for RSC Advances.

SUPPORTING INFORMATION

Hybrid approach to obtain high-quality $BaMO_3$ perovskite nanocrystals

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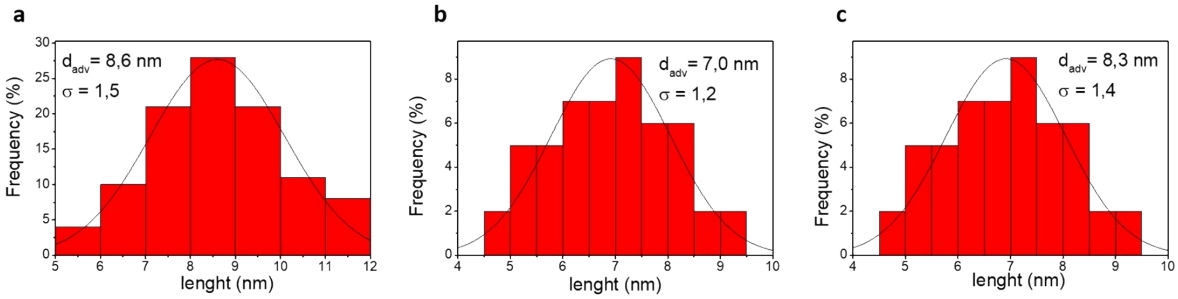


Figure S1. Histogram NCs distribution from the Figure 1 being $BaZrO_3$ (a), $BaHfO_3$ (b) and $BaTiO_3$ (c).

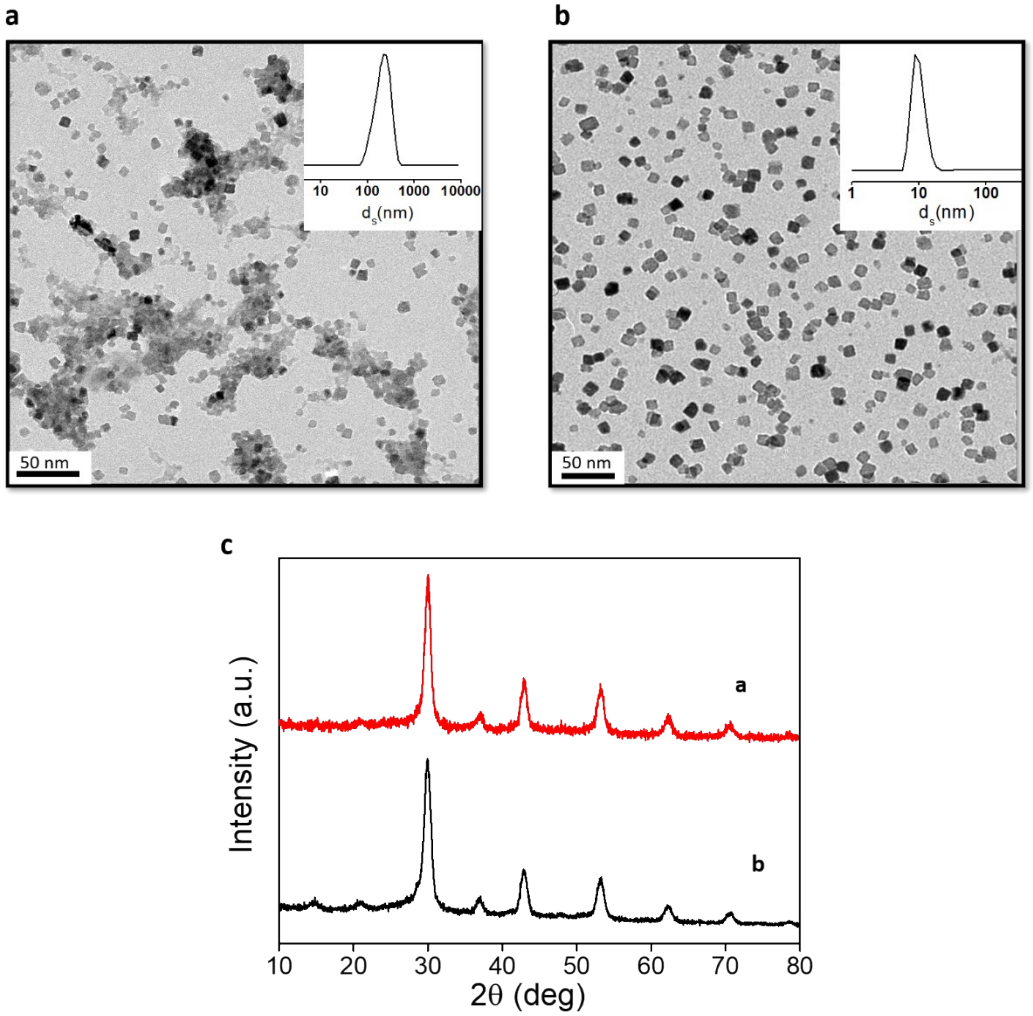


Figure S2. TEM and DLS mesuraments of $BaZrO_3$ NCs at (**a**) stoichiometric Ba:Zr (3.5:3.5 mmol) and (**b**) non-stoichiometric Ba:Zr (3.5:2.8 mmol), (**c**) XRD pattern for stoichiometric (red) on the graph and non-stoichiometric (black), without showing any different phases or impurities.

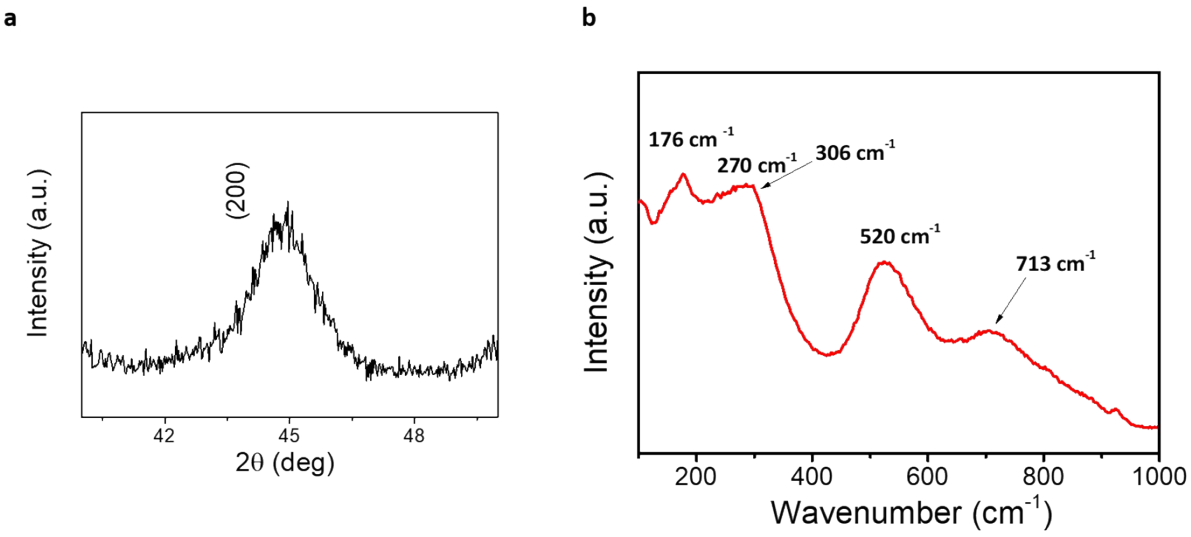


Figure S3 (**a**) XRD zoom on 45 ° of $BaTiO_3$ NCs synthesized at 180 °C for 1 hour, showing the theoretical position where it should be a split peak in a tetragonal phase (b) Raman spectroscopy of $BaTiO_3$ powder at room temperature, without a sign of sharp peak on 306 cm^{-1} and well-defined peak on 713 cm^{-1} as the footprint of the tetragonal phase.

Table S1. Summary of sizes (TEM and Scherrer equation) at different temperatures.

NCs	Temperature (°C)	TEM (nm)	Scherrer size (nm)
$BaZrO_3$	100	-	-
$BaZrO_3$	180	8.6 ± 1.5	8.2
$BaHfO_3$	100	-	-
$BaHfO_3$	180	7.0 ± 1.2	6.8
$BaTiO_3$	100	8.2 ± 1.6	7.4
$BaTiO_3$	180	8.3 ± 1.4	7.8

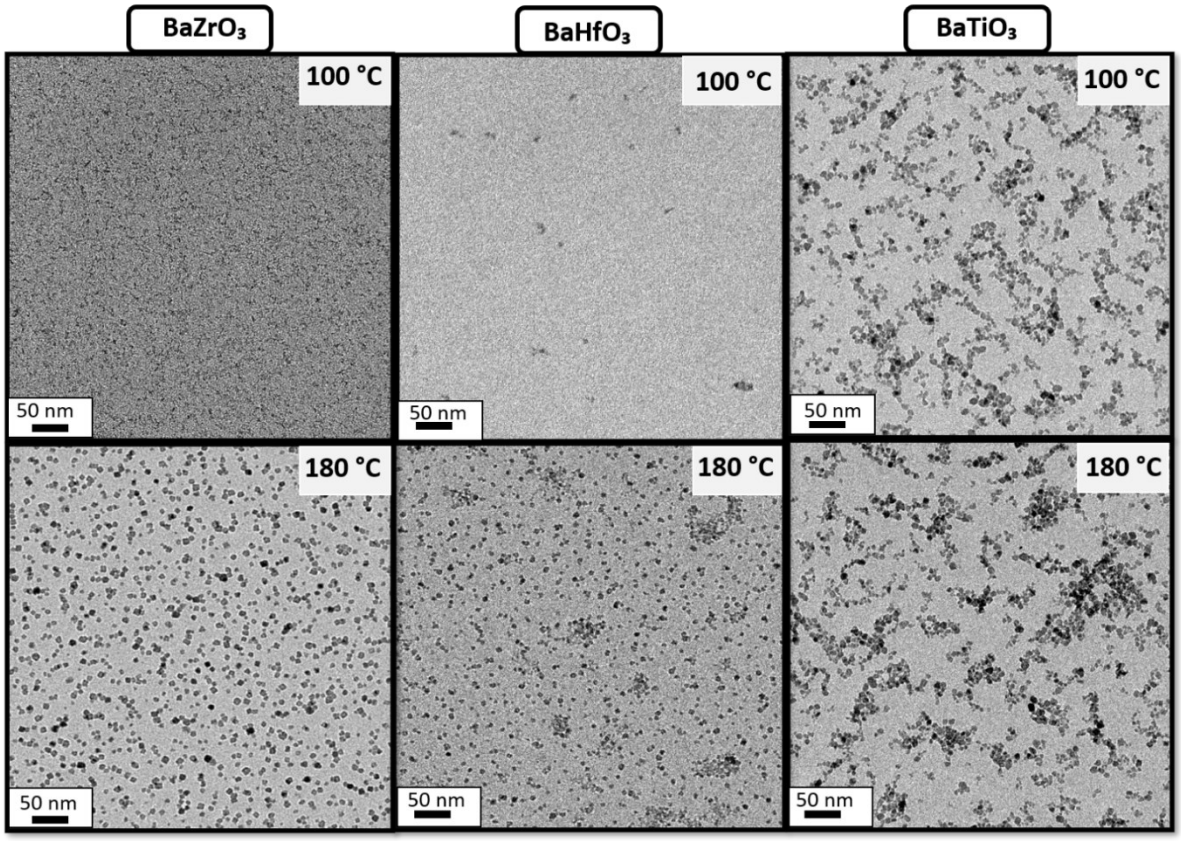


Figure S4. TEM images of $BaZrO_3$, $BaHfO_3$ and $BaTiO_3$ synthesised via standard procedure by using 1 mL of ammonia for 1 hour at 100 and 180 °C.

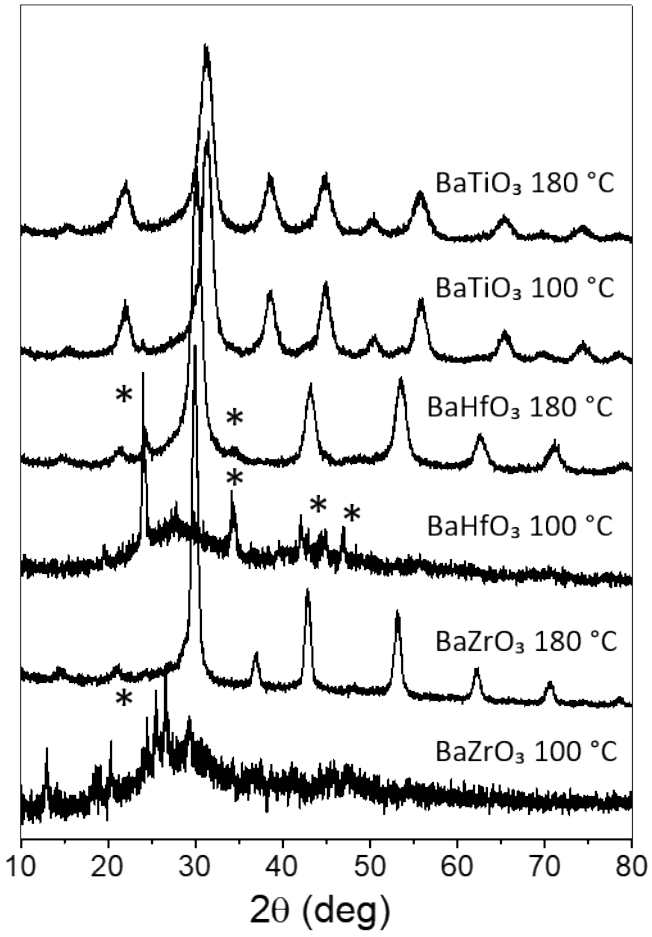


Figure S5. XRD pattern of $BaZrO_3$, $BaHfO_3$ and $BaTiO_3$ synthesized via standard procedure by using 1 mL of ammonia for 1 hour at 100 and 180 °C. In the case of $BaMO_3$ (M = Zr and Hf) at 100 °C the main presence are impurities coming from the *$BaCO_3$ without a final crystal formation. $BaHfO_3$ at 180 °C shows a *$BaCO_3$ peak suggesting a 5% of impurity.

Table S2. TEM and Scherrer size of the three different perovskite NCs at 180 °C for 1 hour and 24 hours of reaction.

NCs	Time (hours)	TEM size (nm)	Scherrer size (nm)
$BaZrO_3$	1	8.6 ± 1.5	8.2
$BaZrO_3$	24	8.8 ± 1.7	8.5
$BaHfO_3$	1	7.0 ± 1.2	6.8
$BaHfO_3$	24	6.8 ± 1.4	6.4
$BaTiO_3$	1	8.3 ± 1.4	7.8
$BaTiO_3$	24	8.0 ± 1.3	7.2

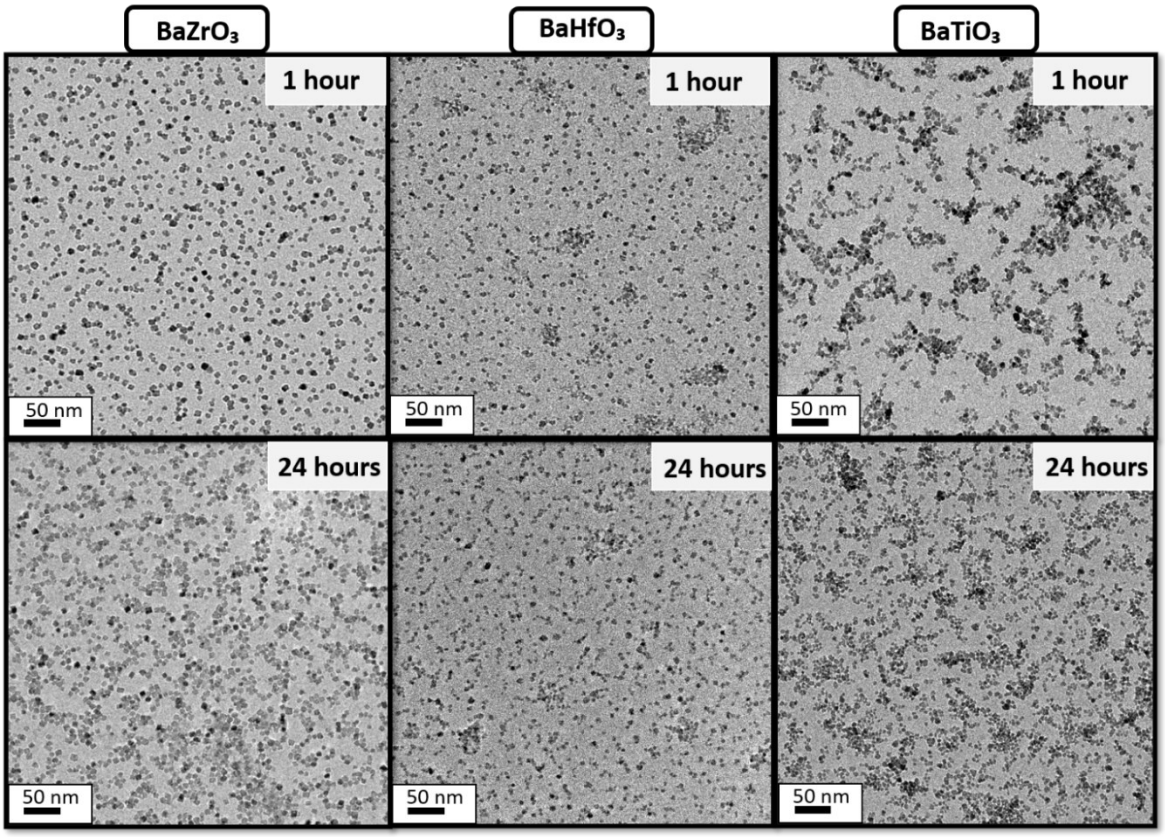


Figure S6. TEM patterns from $BaZrO_3$ and $BaHfO_3$ NCs at 180 °C and $BaTiO_3$ NCs at 100 °C synthesized via standard procedure by using 1 mL of ammonia for 1 hour and 24 hours.

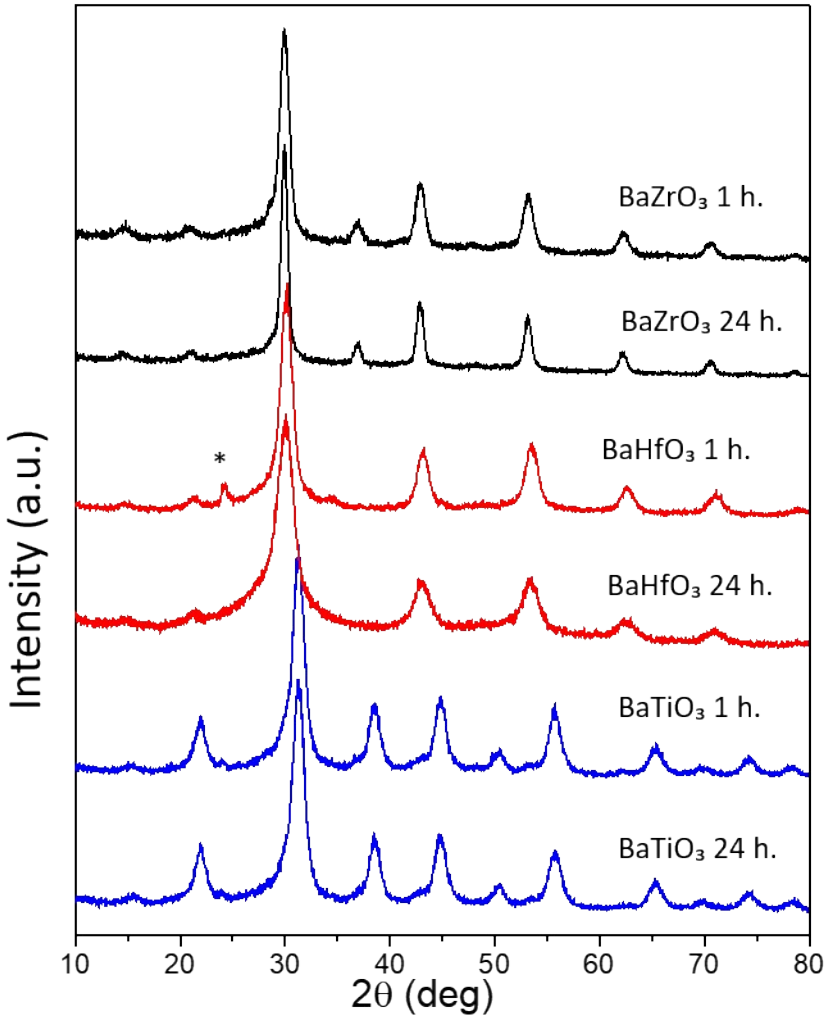
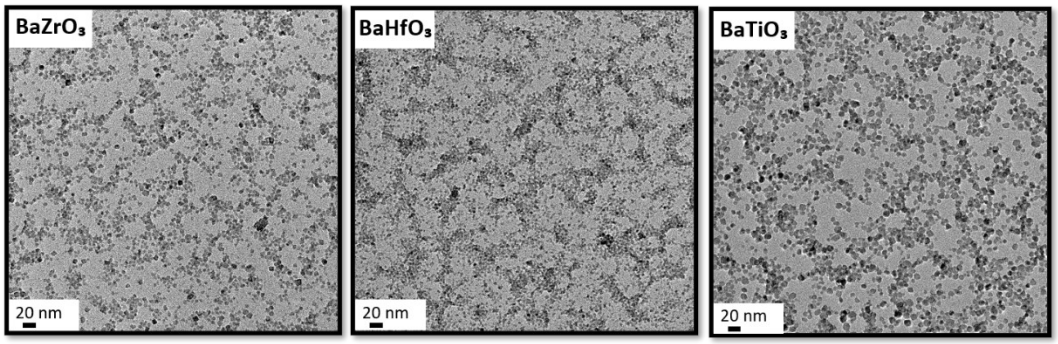


Figure S7. XRD diffraction patterns from $BaZrO_3$ and $BaHfO_3$ NCs at 180 °C and $BaTiO_3$ NCs at 100 °C synthesised via standard procedure by using 1 mL of ammonia for 1 hour and 24 hours. $BaHfO_3$ at 180 °C shows a *$BaCO_3$ peak suggesting a 5% of impurity.

a



b

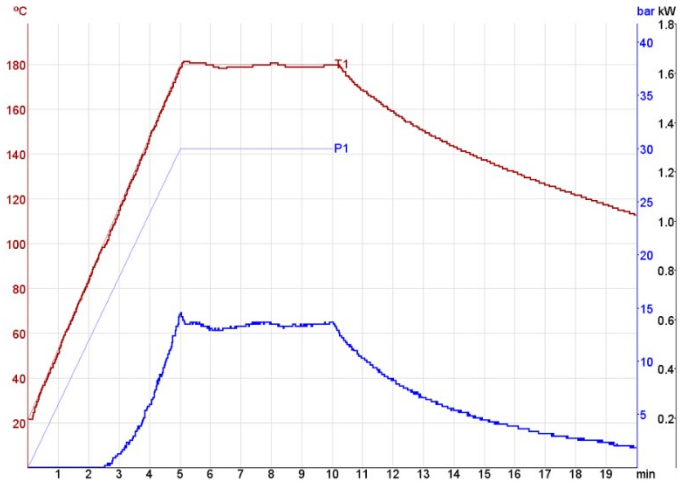


Figure S8. (a) TEM image for $BaZrO_3$, $BaHfO_3$ and $BaTiO_3$ NCs synthesised by using microwave activation, with a ramp of 36 °C/min and dwell during 5 minutes at 180 °C ($BaZrO_3$, $BaHfO_3$) and 100 °C ($BaTiO_3$). The methodology was made using 0.5 mL of H_2O instead of ammonia. (**b**) An example of $BaZrO_3$ microwave profile (temperature and pressure).

Table S3. Table showing TEM and Scherrer sizes using three different metal precursors and the microwave methodology.

Metal precursor	Size TEM (nm)	Scherrer size (nm)
$Zr(OBu)_4$	5.8 ± 1.2	5.3
$Hf(OBu)_4$	4.5 ± 0.8	4.1
$Ti(OBu)_4$	6.3 ± 1.1	5.9

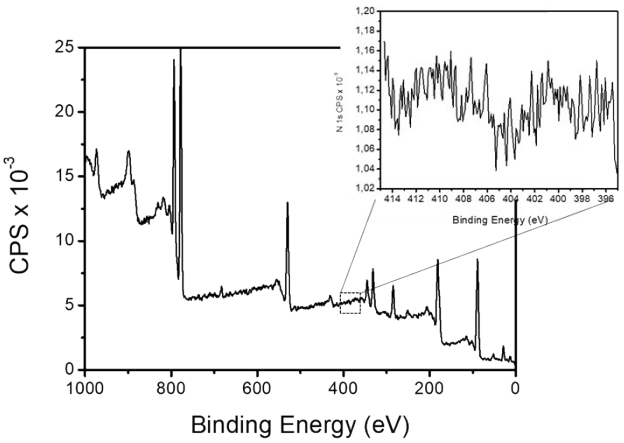


Figure S9. XPS analysis of $BaZrO_3$ NCs synthesized with 1 mL of ammonia at 180 °C for 1 hour. It shows the lack of nitrogen presence on the NC surface.

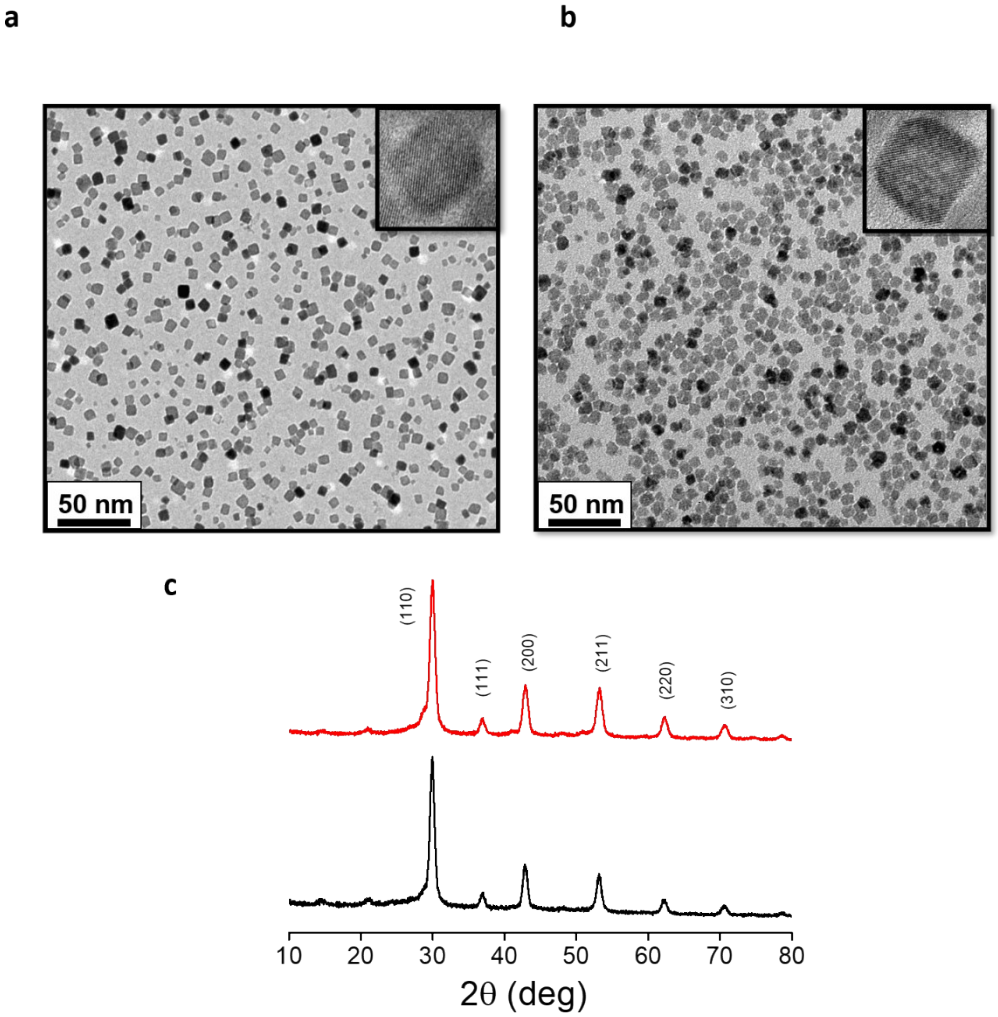


Figure S10. (a) (HR)TEM of $BaZrO_3$ NCs synthesized via standard procedure by using 0.7 mL of water instead of ammonia at 180 °C for 1 hour. (b) (HR)TEM of $BaZrO_3$ NCs synthesized via standard procedure by using 1 mL of ammonia 30% v/v (i.e. 0.3 mL and 0.7 mL water) at 180 °C for 1 hour (c) the respective XRD cubic pattern from (a) black and (b) red.

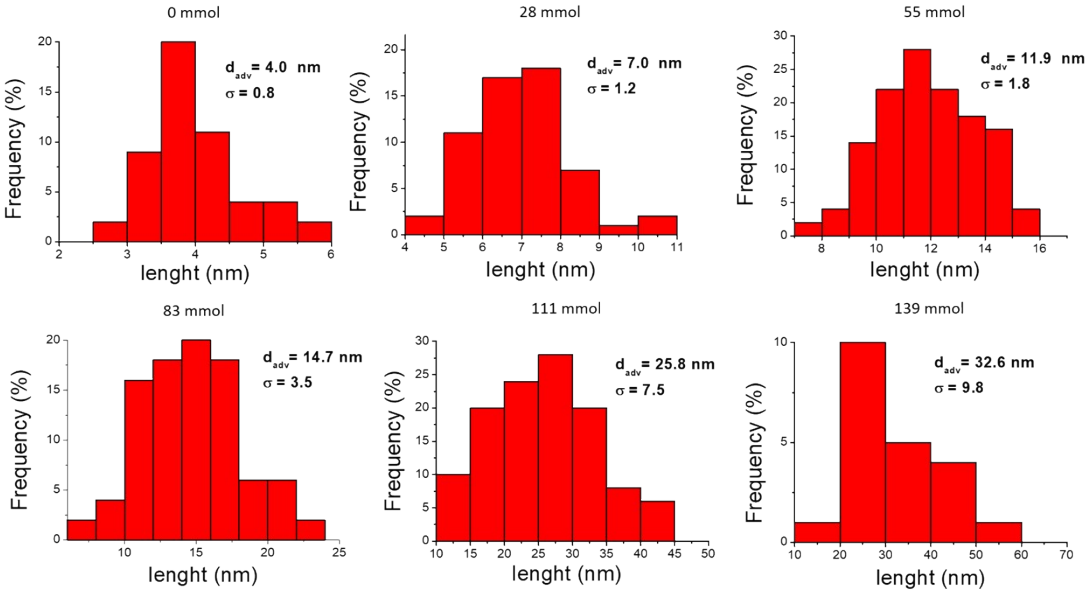


Figure S11. Histograms of the $BaZrO_3$ NCs obtained with different amount of water (0, 28, 55, 83, 111 and 139 mmol) corresponding to TEM images in Figure 3.

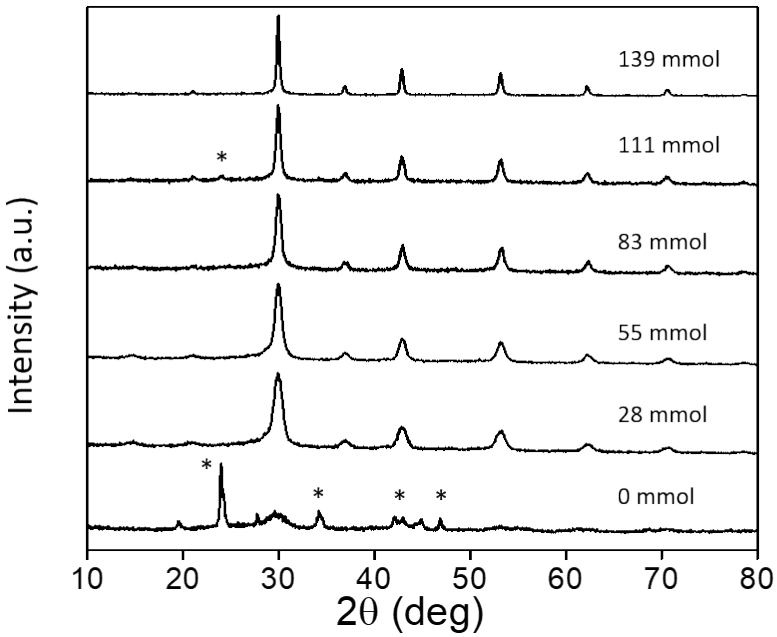


Figure S12. XRD pattern corresponding to the NCs showed in Figure 3 for the different amounts of water from 0 mmol to 139 mmol. XRD at 0 mmol also includes the main peaks of *$BaCO_3$ as the main impurity of this synthesis. 111 mmol pattern also shows a subtle *$BaCO_3$ peak suggesting an impurity quantification of 4% from $BaCO_3$.

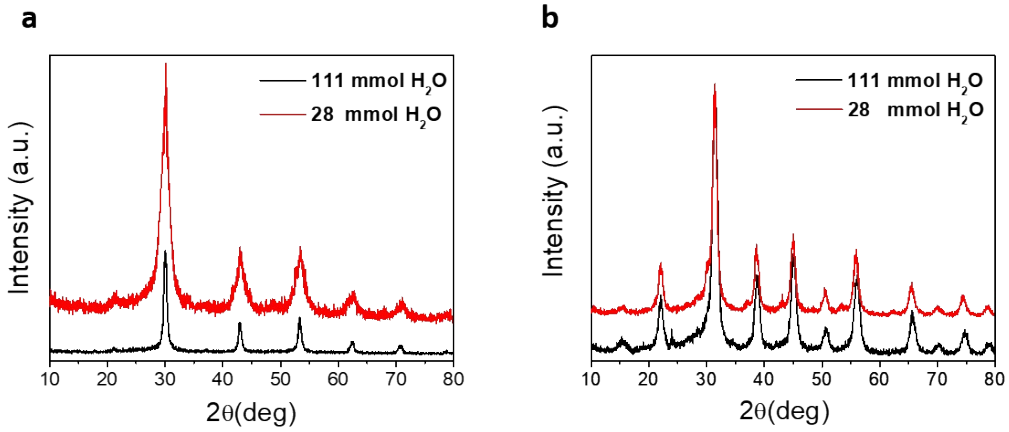


Figure S13. XRD diffraction patterns for (a) $BaHfO_3$ and (b) $BaTiO_3$ NCs synthesised via standard procedure by adding 28 and 111 mmols of water instead of ammonia at 180 °C ($BaHfO_3$) and at 100 °C ($BaTiO_3$).