

# Calcite Nanocrystals Investigated using X-ray Absorption Spectroscopy

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**Table S1: Crystallographic data obtained from Rietveld refinement**

	CNS 1	CNS 2	CNS 3
Formula weight	100.0869	100.0869	100.0869
Crystal system	Trigonal	Trigonal	Trigonal
Space group	$R\bar{3}c$	$R\bar{3}c$	$R\bar{3}c$
$a$ (Å)	4.98352(26)	4.99026(17)	4.98898(16)
$b$ (Å)	4.98352(26)	4.99026(17)	4.98898(16)
$c$ (Å)	17.1297(14)	17.1438(9)	17.1223(8)
V	368.428(28)	369.730(18)	369.075(17)
wRp	10.21	12.56	11.11
Rp	8.25	9.49	8.46
Chi <sup>2</sup> ( $\chi^2$ )	1.21	3.28	2.61

**Table S2: Bands observed in the FTIR spectra of calcite nanocrystals**

Nanocrystals		FTIR Bands (cm <sup>-1</sup> )	
CNS1	873	712	636
CNS2	872	712	638
CNS3	874	712	639

**Table S3. Main edge, E<sub>o</sub> and positions of spectral features A<sub>1</sub>, A<sub>2</sub>, A<sub>3</sub>, A<sub>4</sub> and in eV for different nanocrystals**

Nanocrystals	E <sub>o</sub>	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	A <sub>4</sub>
CNS1	4042.7±0.4	4049.4±0.4	4060.9±0.4	4078.4±0.4	4093.4±0.4
CNS2	4042.6±0.4	4049.4±0.4	4060.9±0.4	4078.4±0.4	4093.4±0.4
CNS3	4042.8±0.4	4049.4±0.4	4060.9±0.4	4078.4±0.4	4093.4±0.4

**Table S4.** Coordination number (*N*), Bond-distance (*R*), Debye-Waller factor ( $\sigma^2$ ), energy-correction ( $\epsilon_0$ ) and R-factor for calcite nanocrystals.

Nanocrystals	Shell	<i>N</i>	<i>R</i> (Å)	$\sigma^2$ (Å <sup>2</sup> )	$\epsilon_0$ (eV)	<i>R</i> -Factor
<b>CNS1</b>	Ca-O	5.7	2.39	0.004*	6.74*	0.03
	Ca-Ca	4.1	3.13	0.026*		
<b>CNS2</b>	Ca-O	5.1	2.28	0.004*	-4.533*	0.02
	Ca-Ca	6.6	2.93	0.003		
<b>CNS3</b>	Ca-O	5.4	2.27	0.005*	-3.73*	0.03
	Ca-Ca	6.5	2.97	0.004*		
<b>Std</b>	Ca-O	6	2.35			
	Ca-Ca	6	3.15			

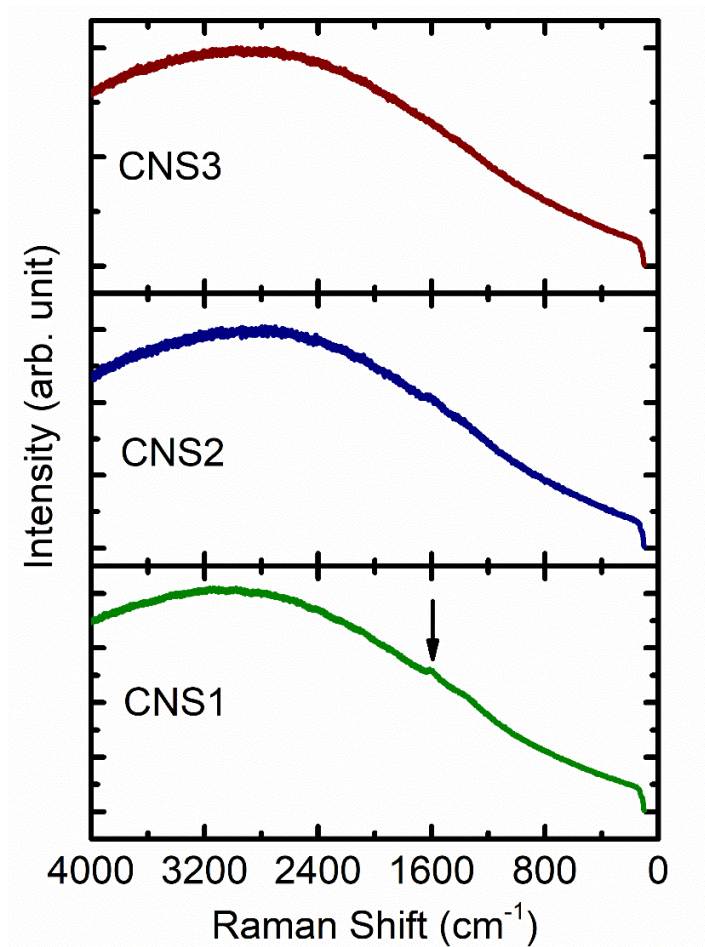
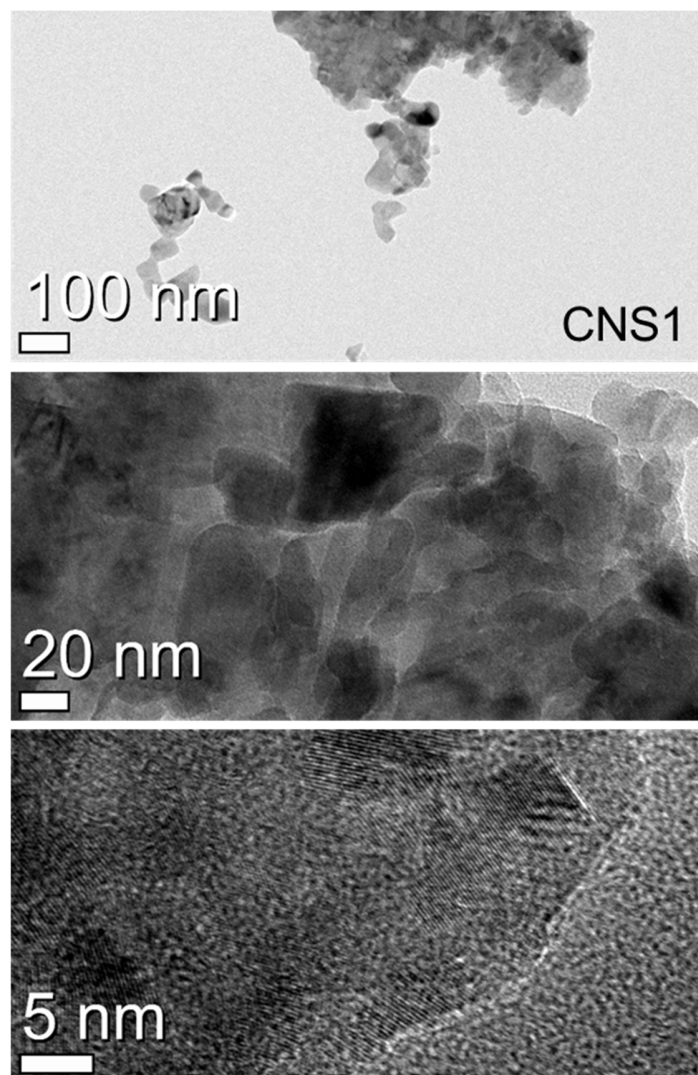
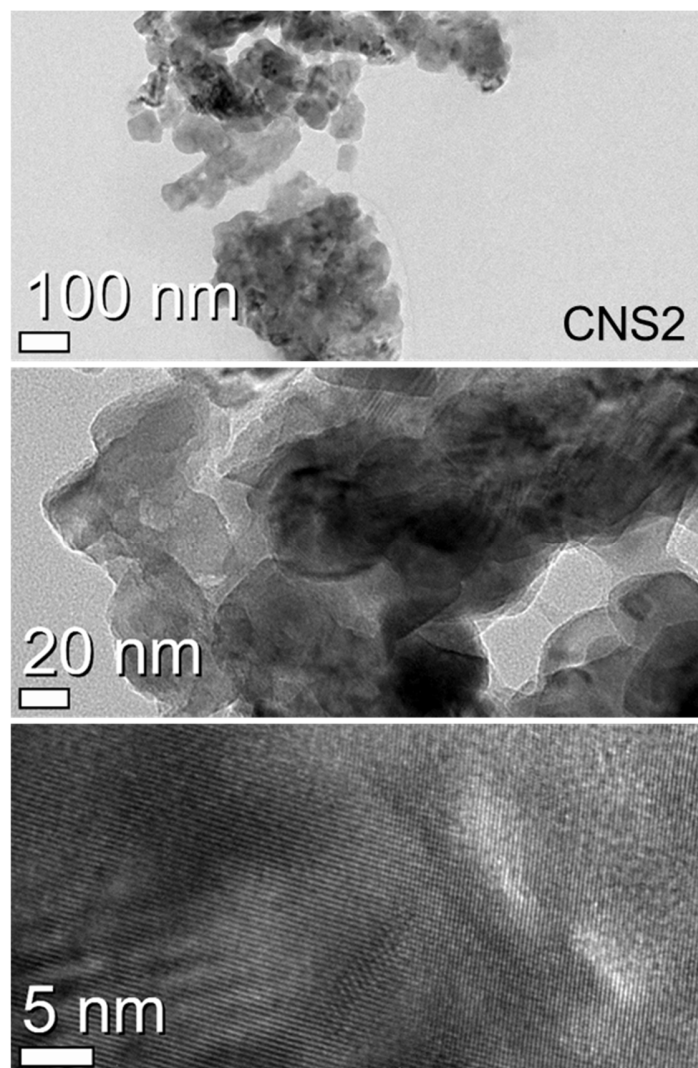


Figure S1: Raman Spectra of CNS1, CNS2 and CNS3

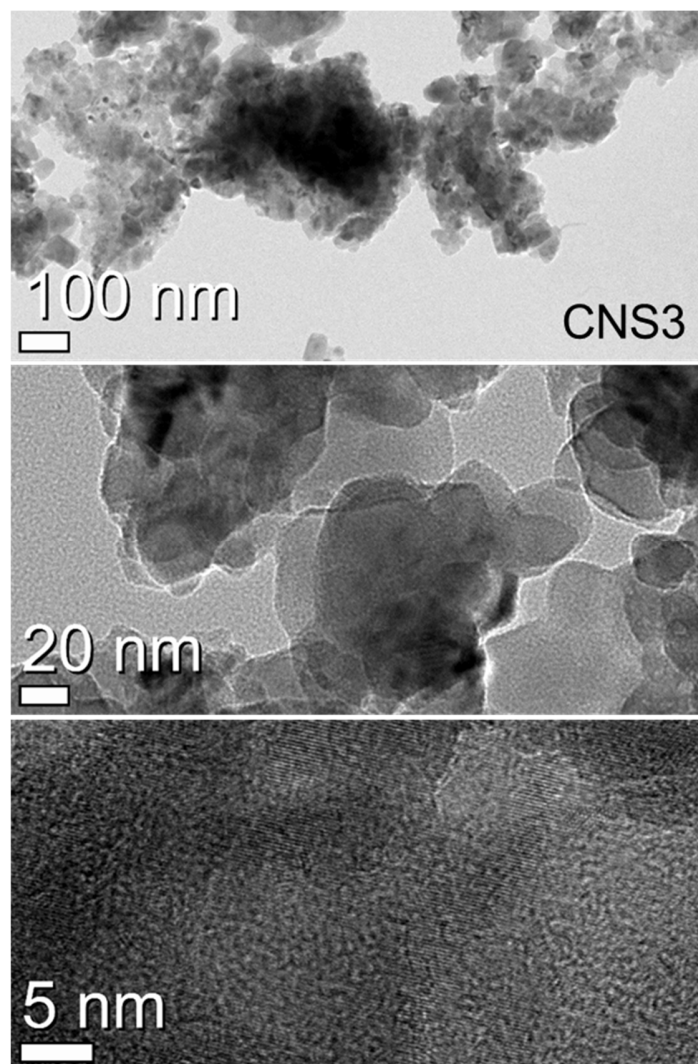


**Figure S2:** TEM micrographs of CNS1 at different magnifications



**Figure S3:** TEM micrographs of CNS2 at different magnifications





**Figure S4:** TEM micrographs of CNS3 at different magnifications

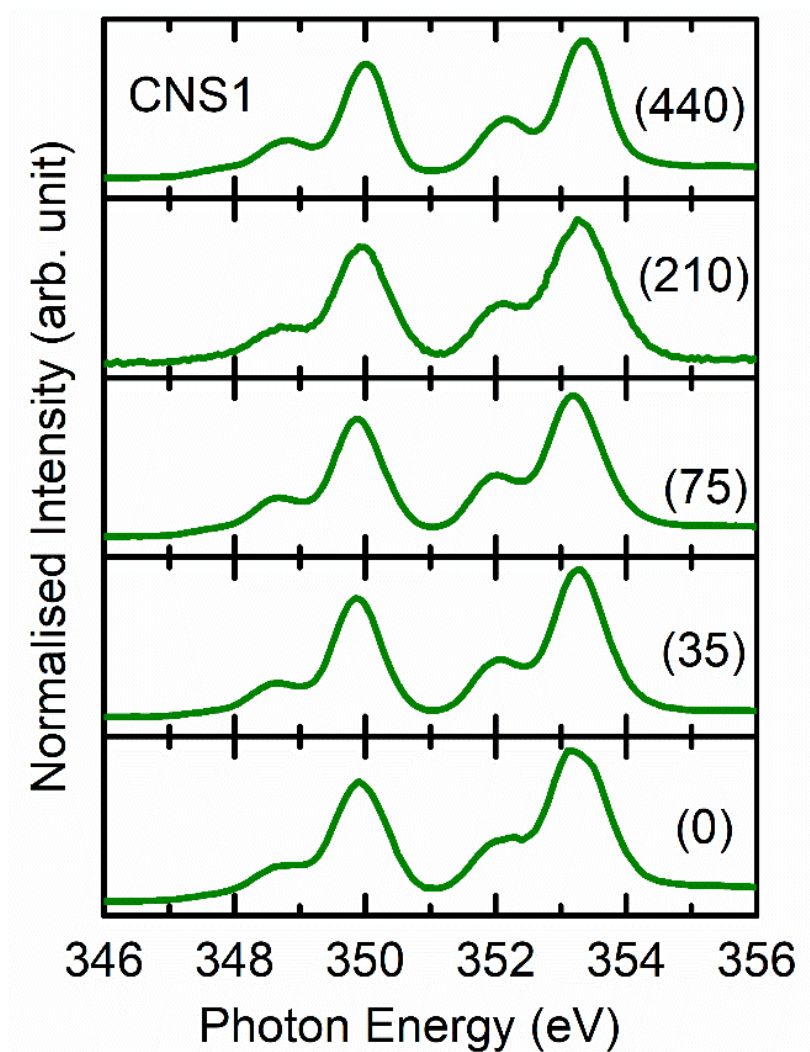
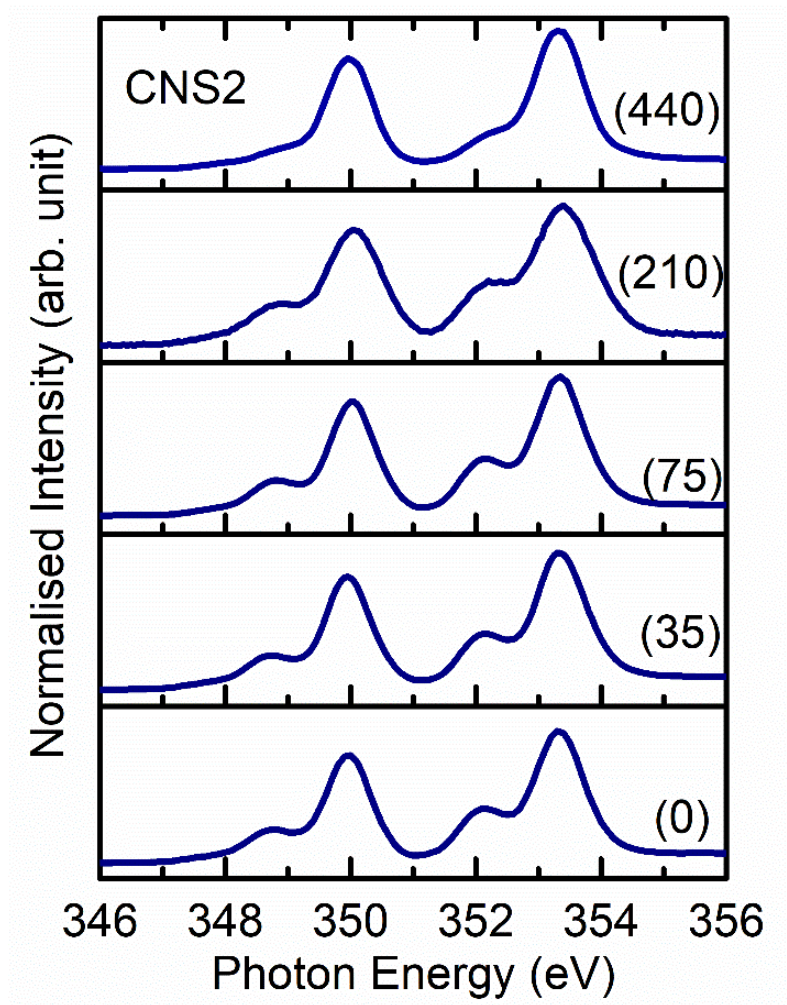
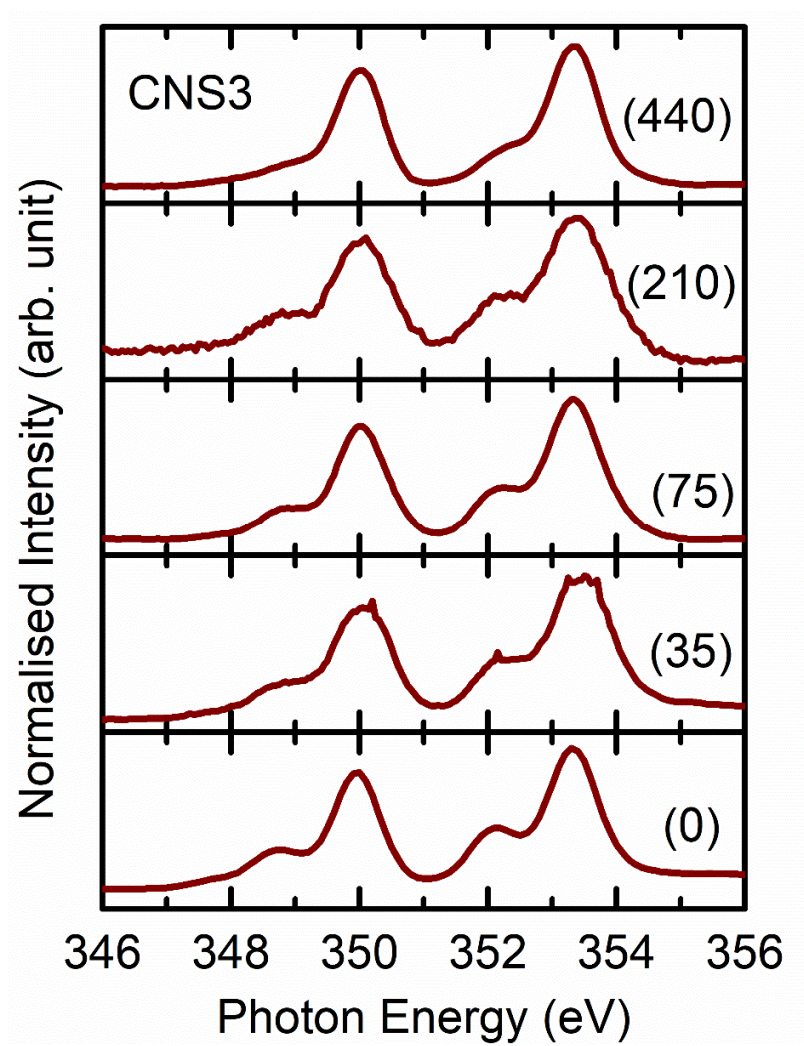


Figure S5: Ca *L*-edge spectra measured at different durations for CNS1



**Figure S6:** Ca *L*-edge spectra measured at different duration for CNS2



**Figure S7:** Ca *L*-edge spectra measured at different duration for CNS3