

Electronic Supplementary Information (ESI)

Tunable Structural and Optical Properties of CuInS₂ Colloidal Quantum Dots as Photovoltaic Absorbers

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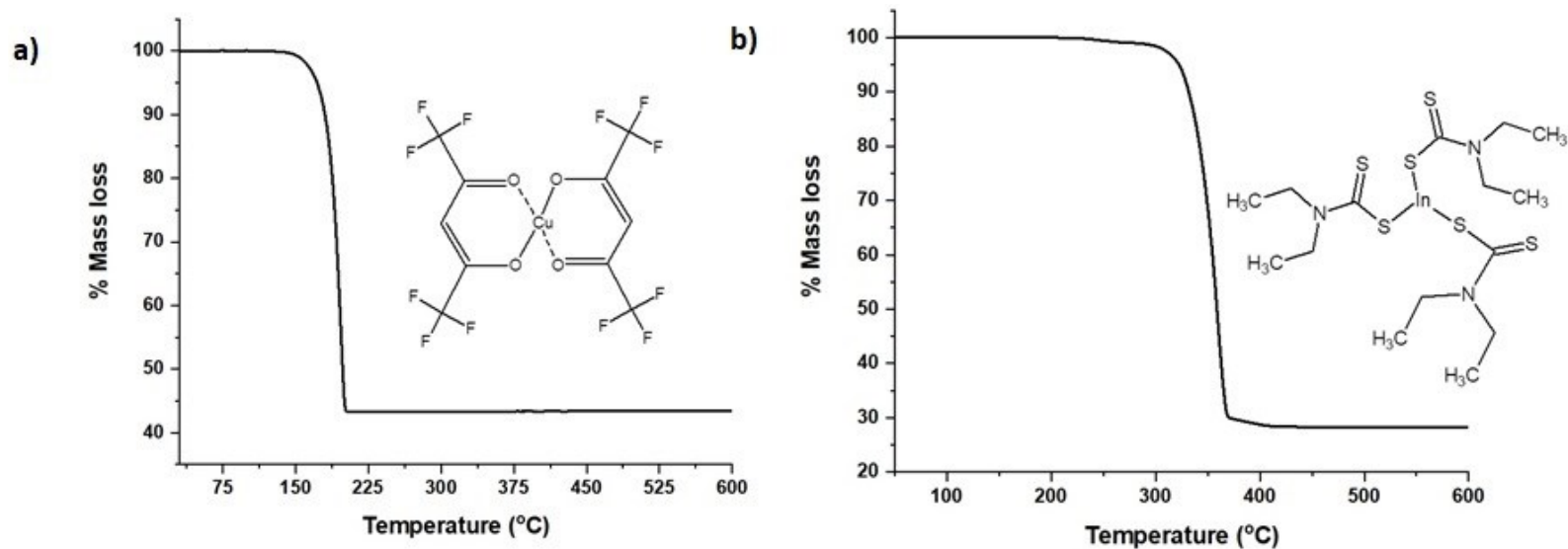


Figure S1: TGA thermograms for a) Cu(Hfacac)₂.xH₂O b) In(dedtc)₃ with respective molecular structures.

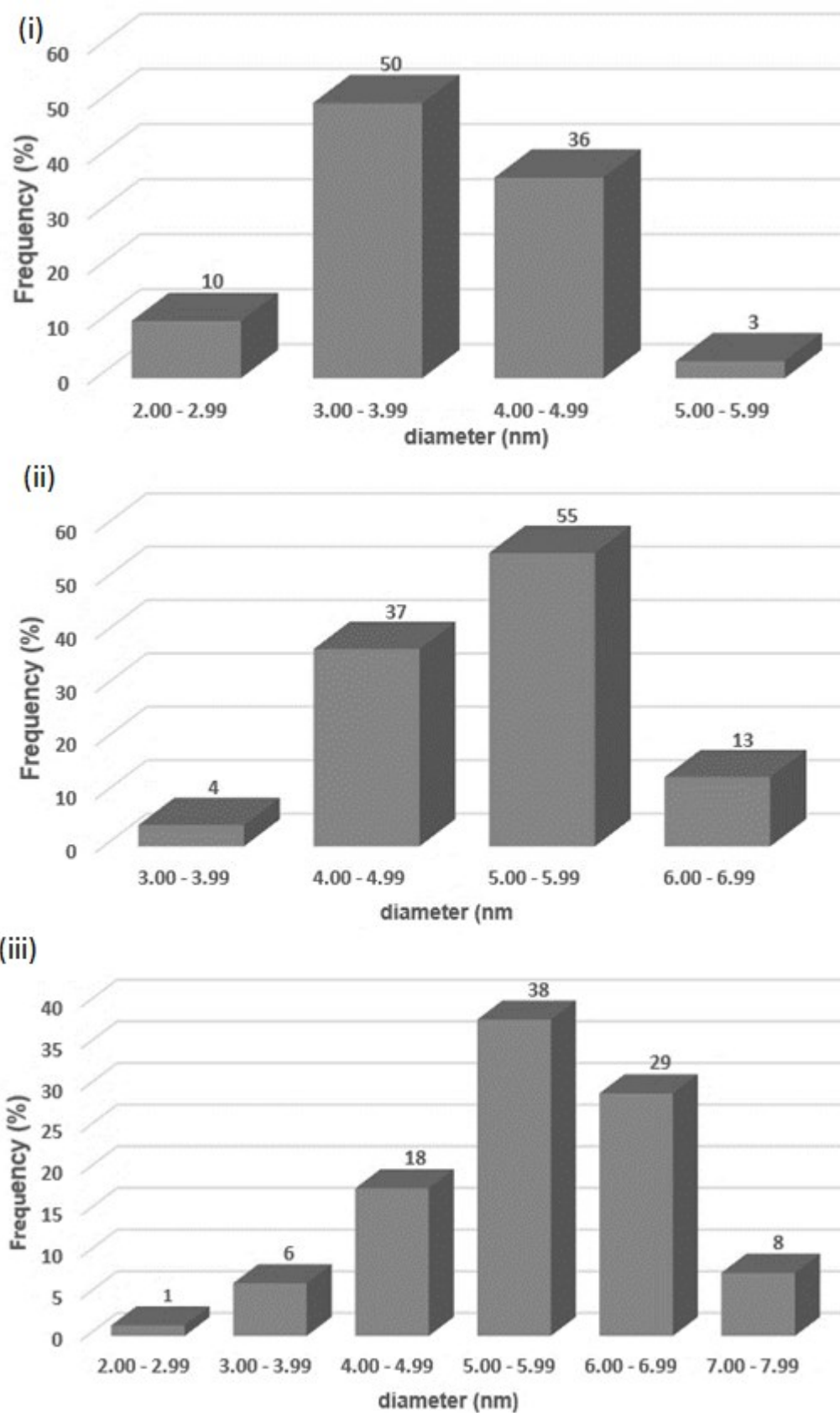


Figure S2: Histograms showing size distribution from TEM of CIS nanoparticles synthesized at (i) 140, (ii) 180 and (iii) 210 °C, respectively for 60 minutes.

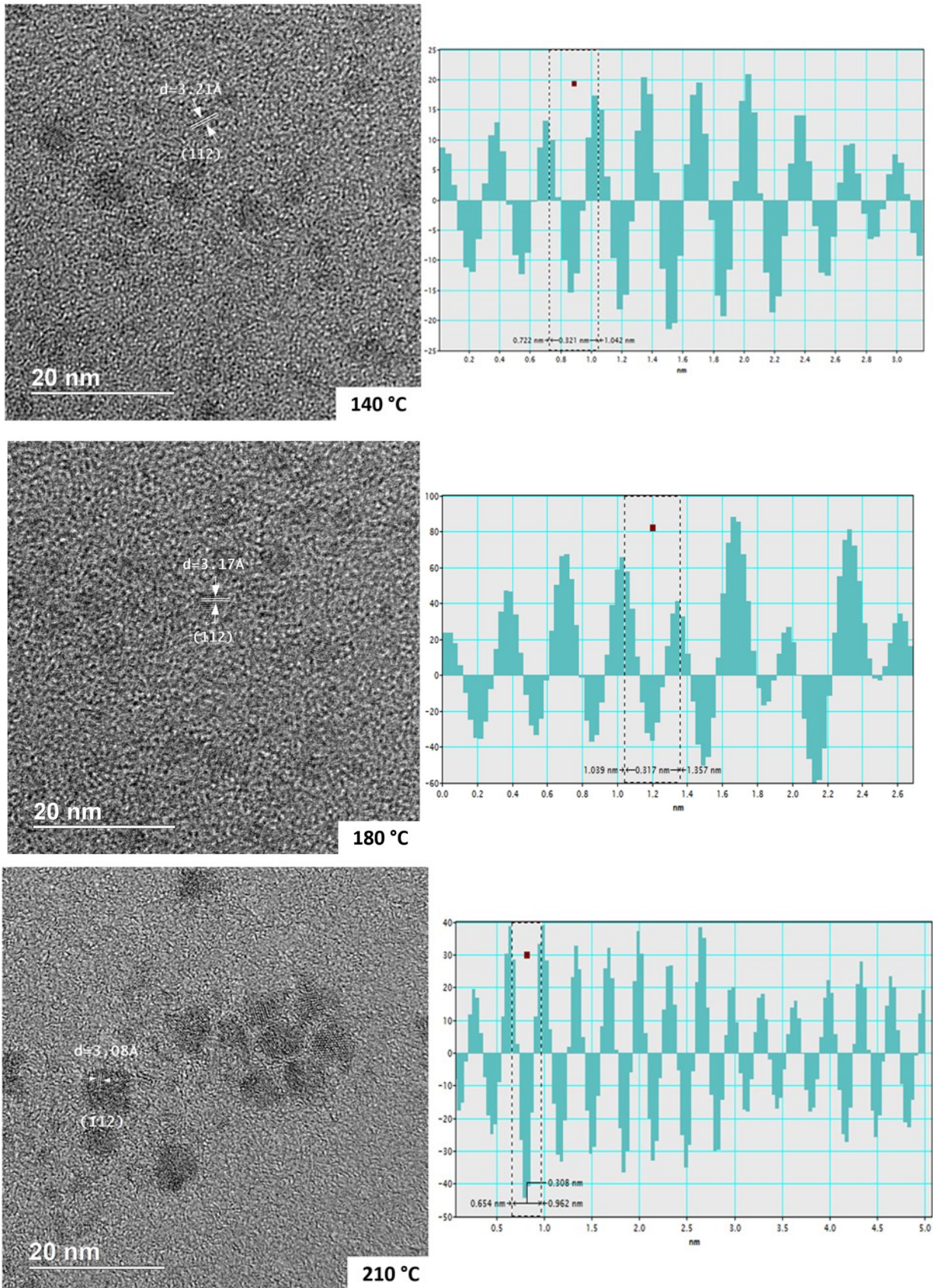


Figure S3: (Left) HR-TEM images of nanoparticle ensemble at different reaction temperatures with inset highlighting lattice spacings (right) corresponding lattice spacing measurements of 3.21, 3.17 and 3.08 Å.

Table S1: Lattice parameters, hkl values and corresponding d-spacings of synthesized chalcopyrite and wurtzite nanoparticles.

Crystal Lattice: Tetragonal		
Space Group I-42d		
a = b = 5.5230, c = 11.14		
$\alpha = \beta = \gamma = 90^\circ$		
hkl	d-spacing	2theta
112	3.22541	27.634
204/220	1.94654	46.6228
116/312	1.65718	55.3979
Crystal Lattice: Hexagonal		
Space Group P63mc		
a = b = 3.9065, c = 6.4290		
$\alpha = \beta = 90^\circ$ and $\gamma = 120^\circ$		
hkl	d-spacing	2theta
100/002	3.32337	26.8041
101	3.00959	29.6595
102	2.31923	38.7969
110	1.95491	46.4113
103	1.81526	50.2186
112	1.66885	54.9776
203	1.33012	70.7776
211	1.255	75.727

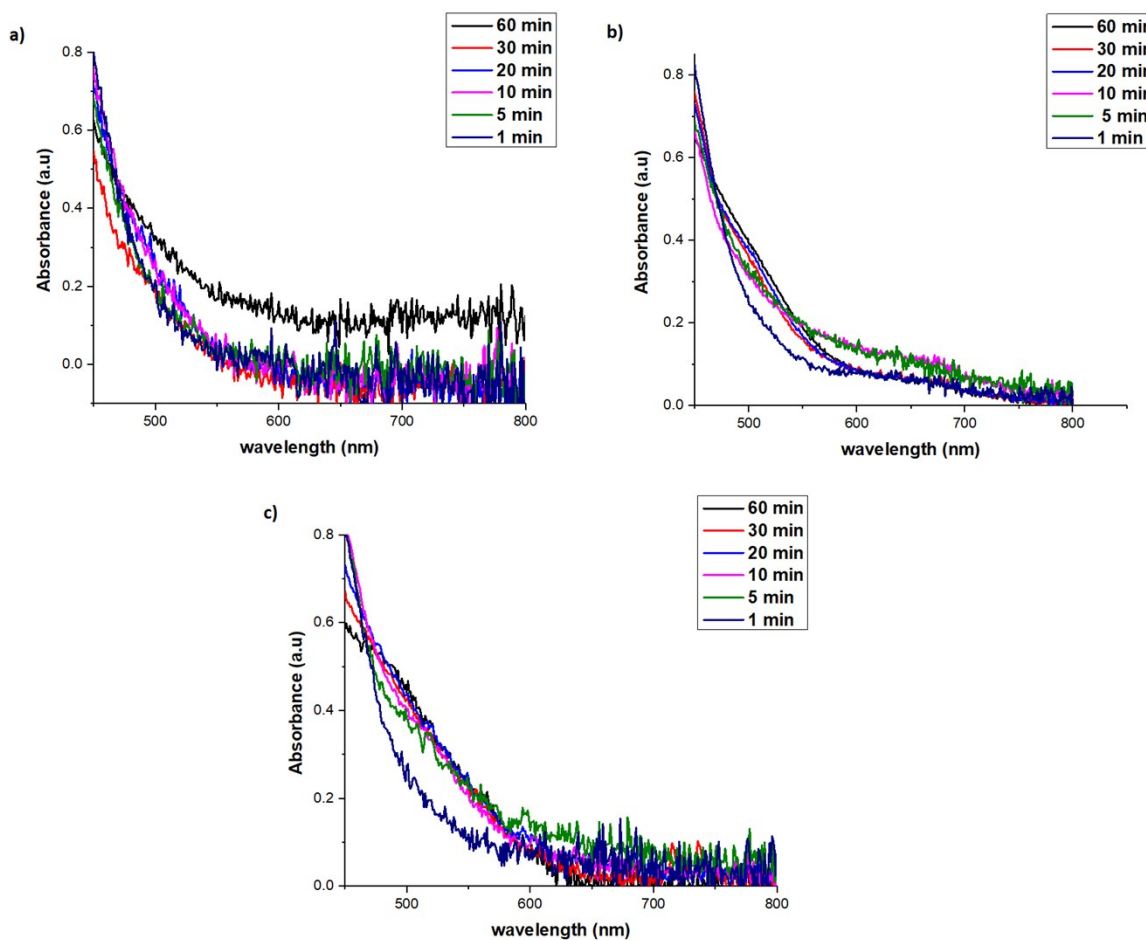


Figure S4: UV-vis absorption spectra of aliquots taken at specific intervals from reactions at temperatures a) 140 b) 180 c) 210 °C, respectively.

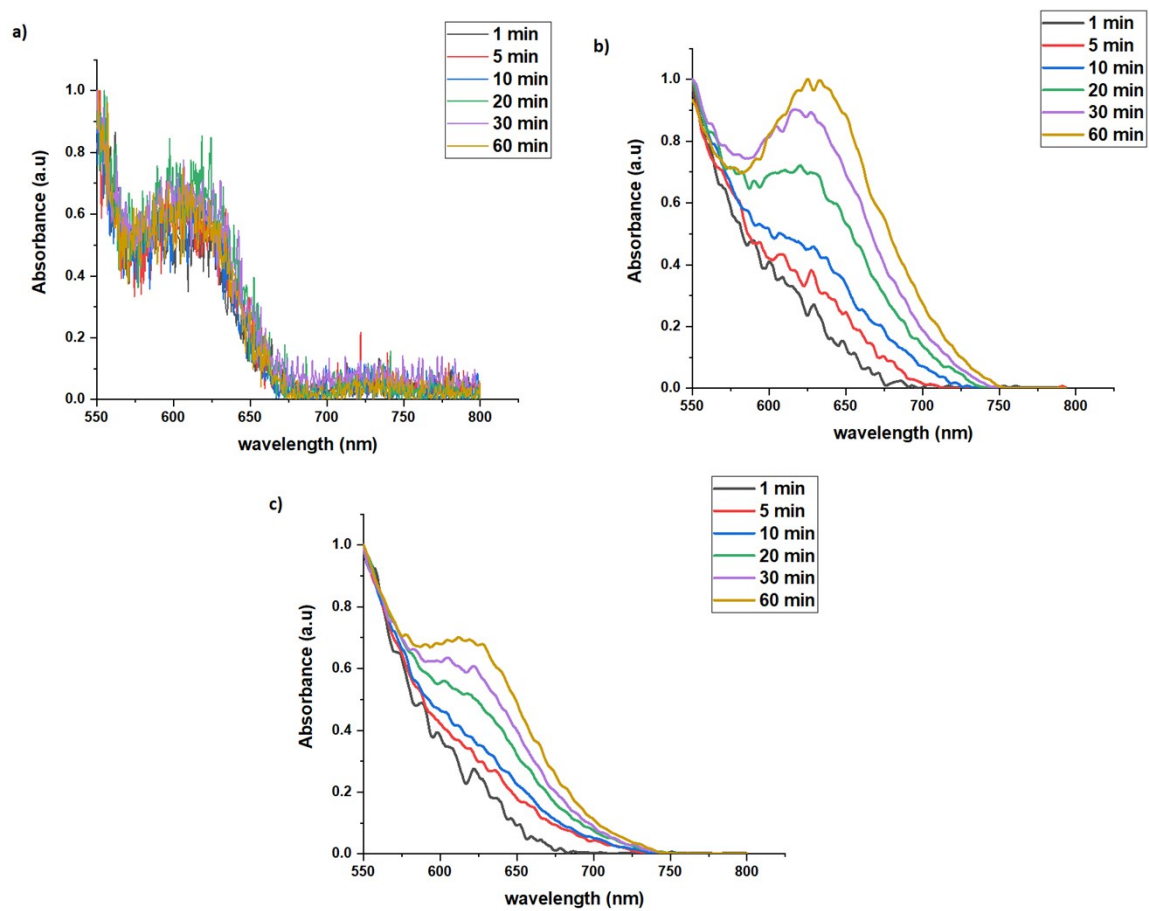


Figure S5: Photoluminescence spectra of aliquots taken at specific intervals from reactions at temperatures a) 140 b) 180 c) 210 °C ($\lambda_{\text{exc}} = 440$ nm).