Supporting Information

Thermodynamic Control of Iron Pyrite Nanocrystal Synthesis with High Photoactivity and Stability

Alec Kirkeminde and Shenqiang Ren*

Department of Chemistry, University of Kansas, Lawrence, Kansas 66045, United States

Materials:

All materials were used as received. For synthesis of crystals, FeCl₂ (99.9%), Octadecylamine (90% technical grade), Sulfur powder, Diphenyl Ether(99% reagent grade)were all obtained from Sigma Aldrich. For washing the particles Chlorophorm (99% anhydrous) was obtained from EMD and Methanol (99.8%) from VWR. Methyl orange used in photocatalytic experiments was obtained from Fluka Chemical.

XRD Data Collection/Analysis:

Three overlapping 1 minute 180° φ -scans were collected using the Bruker Apex2 V2010.3-0 software package with the detector at $2\theta = 30^{\circ}$, 60° and 90° using a sample-to-detector distance of 50.0 mm. These overlapping scans were merged and converted to a .RAW file using the Pilot/XRD2 evaluation option that is part of the APEX2 software package. This .RAW file was then processed using the Bruker EVA powder diffraction software package.



Figure S1: SEM images of FeS₂ nanocubes (120°C synthesis), popcorns (170°C synthesis) and nano spheres (120°C synthesis) of FeCl₂ precursor.



Figure S2: TEM images of seed's at 5 min into reaction of $FeCl_2$ precursor at (a) 220°C synthesis showing that the seeds start as Quantum dots and (b) 120°C synthesis the seeds start as cubes.



Figure S3: Methyl orange degradation spectra results for (a) cubes, (b) popcorn, (c) nano spheres, (d) thin sheets, (e) thick sheets. Absorbance at λ_{max} vs. time (min) for all samples presented in (f).



Figure S4: TEM image of FeS_2 Nano-Spheres after photocatalytic experiment. It can be seen that the particles to extent degrade during the process, which is also shown by the shift in the absorbance peak, but remain mostly intact.