

Supplementary Information for

Origin of Photocarrier Losses in Iron Pyrite (FeS₂) Nanocubes

*Sudhanshu Shukla^{1, 2}, Guichuan Xing³, Hu Ge², Rajiv Ramanujam Prabhakar⁴, Sinu Mathew⁵,
Zhenghua Su⁴, Venkatram Nalla⁶, Thirumalai Venkatesan⁵, Nripan Mathews², Thirumany
Sritharan², Tze Chien Sum³ and Qihua Xiong,^{3, 7}*

¹Energy Research Institute, Interdisciplinary Graduate School, ²School of Materials Science and Engineering, Nanyang Technological University, Singapore, ³Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore, ⁴Energy Research Institute, Nanyang Technological University, Singapore
⁵Department of Electrical and Computer Engineering, National University of Singapore, Singapore 117576, NUSNNI-NanoCore, National University of Singapore, Singapore 117576,
⁶Centre for Disruptive Photonic Technologies (CDPT), Nanyang Technological University, Singapore 639798 and ⁷NOVITAS, Nanoelectronics Centre of Excellence, School of Electrical and Electronic Engineering, Nanyang Technological University, Singapore

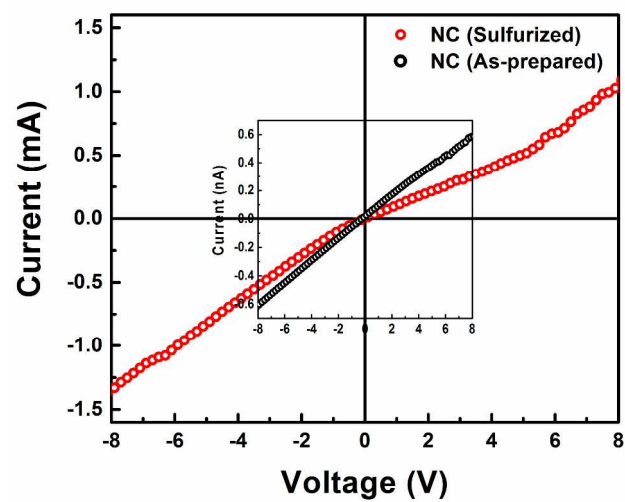


Figure S1 Current voltage characteristics of as-prepared (central) and sulfurized iron pyrite nanocube thin films

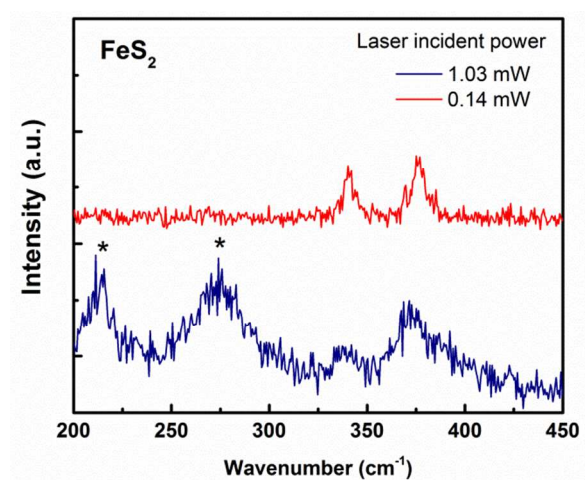


Figure S2 Raman spectra of iron pyrite nanocubes using excitation wavelength of 532 nm, 1.03 mW incident power results in extra peaks (asterisk) due to laser induced oxidation.

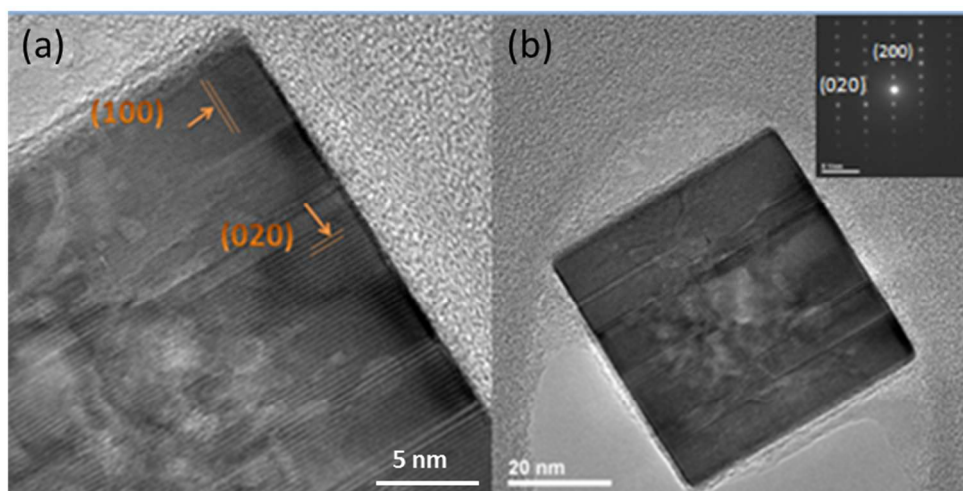


Figure S3 (a) HRTEM image of the edge of as-prepared iron pyrite nanocube, (b) single nanocube, inset shows the FFT pattern of the corresponding lattice fringes

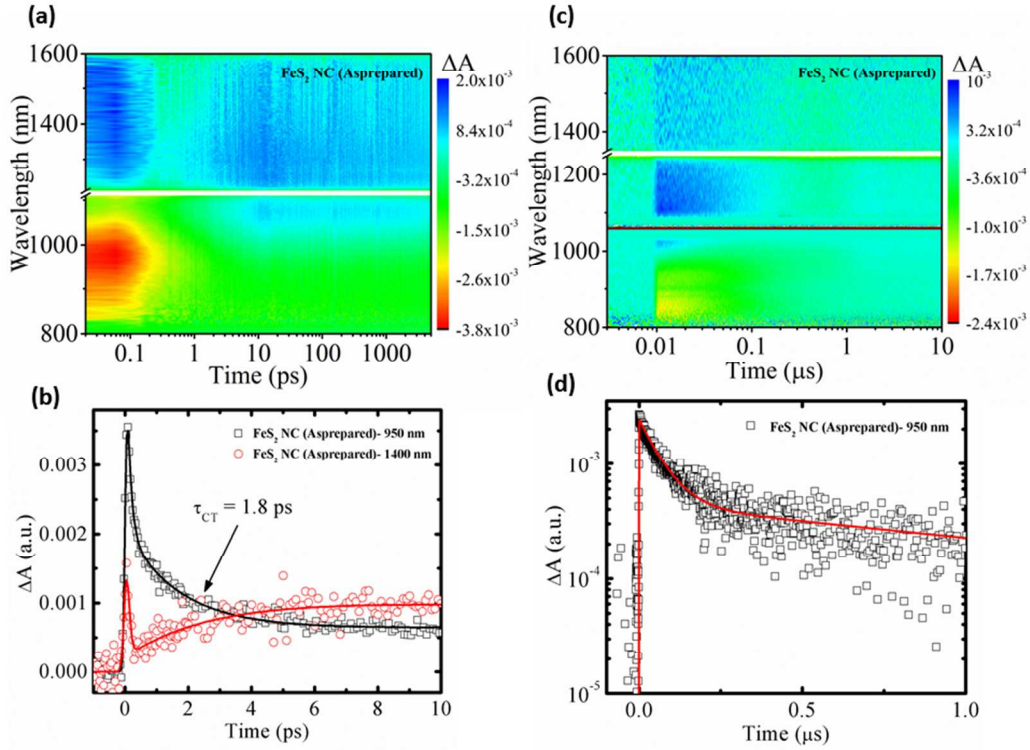


Figure S4 Differential transient absorption spectra after photoexcitation of as-prepared iron pyrite nanocubes as a function of time delay in (a) femto-pico second range, (c) nano-micro second range. Carrier decay dynamics probed at 950 nm (photobleaching) and 1400 nm (photoinduced absorption) by fitting the transients in (b) picosecond range, fitted with single exponential decay function (solid black line) with decay time constant (charge transfer time, τ_{ct}) 1.8 ps and (d) microsecond range, fitted with biexponential decay function with time constants 50 ns (τ_{d1}) and 990 ns (τ_{d2}) associated with long live trap states and eventual recombination process

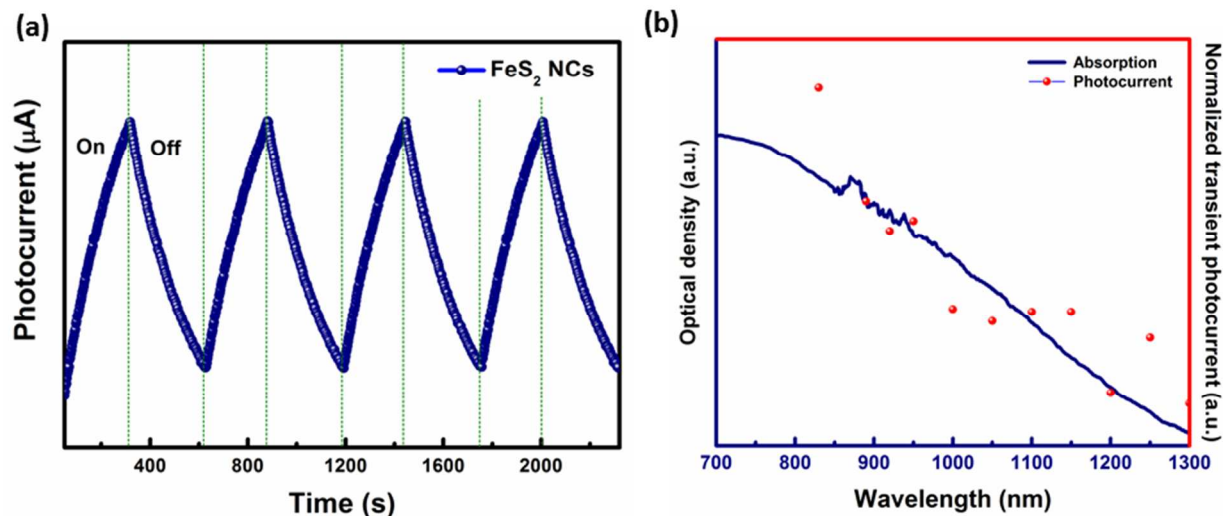


Figure S5 (a) Time dependent photoresponse of iron pyrite nanocubes under broadband white light illumination, measured in a two electrode configuration. (b) Photocurrent measured from femtosecond transient photocurrent spectroscopy (on right) and absorption spectra (on left) of pyrite.

Table ST1. Raw data of the Hall measurement

Probes Source meter	13 24	24 31	13 24	24 31
Current 1 (A)	1.24×10^{-5}	1.24×10^{-5}	1.24×10^{-5}	1.24×10^{-5}
Voltage 1 (V)	-0.10	0.10	-0.10	0.10
Current 2 (A)	-1.24×10^{-5}	-1.24×10^{-5}	-1.24×10^{-5}	-1.24×10^{-5}
Voltage 2 (V)	0.105	-0.106	0.106	-0.106
Resistance (Ohm)	-8485.8	8581.0	-8554.4	8647.2
Field (G)	5016		-5025	

Temperature(K)	302.0
Resistivity ($\Omega \cdot \text{cm}$)	11.20
Mobility ($\text{cm}^2/\text{V}\cdot\text{s}$)	0.10
Density (cm^{-3})	5.30×10^{18}
Hall Coefficient (cm^3/coul)	1.17
Type of carriers	holes