

Graphical Excellence in Scientific Presentations and Papers

Constance Biegel and Prashant V. Kamat
University of Notre Dame

Disclaimer: The views presented here are based on our opinion and does not represent the publication policy of any specific journal. The graphs cited in this presentation have not been cited deliberately to avoid any specific criticisms of a publication. These are presented only as examples. -C. Biegel and P. Kamat

Graphical Excellence*

- Is the well-designed presentation of interesting data – a matter of *substance*, of *statistics*, and of *design*
- Consists of complex ideas communicated with **clarity, precision, and efficiency**

*pg. 51, Tufte, Edward R. *The Visual Display of Quantitative Information*; Graphics Press: Cheshire, CT, 1983; pp 1-197.

Graphical Excellence*

- Is that which gives to the viewer the greatest number of ideas in the shortest time with the least ink in the smallest space
- Is nearly always multivariate
- Requires telling the truth about the data

*pg. 51, Tufte.

What are Good Graphics?

Graphics that communicate ideas with:

- **Clarity**

- Lack of ambiguity and confusion

- **Precision**

- Truthful results
- Distortion-free presentation

- **Efficiency**

- Minimal “chartjunk”

1. Figure Captions

How to phrase good figure captions?

- Describe “(Vertical axis quantity) vs. (Horizontal axis quantity)” for Experiment
- Include all important experimental details
- Identify multiple curves or traces
- Match the graphic

Describe what is graphed

“(Vertical axis quantity) vs. (horizontal axis quantity) for (experiment)”

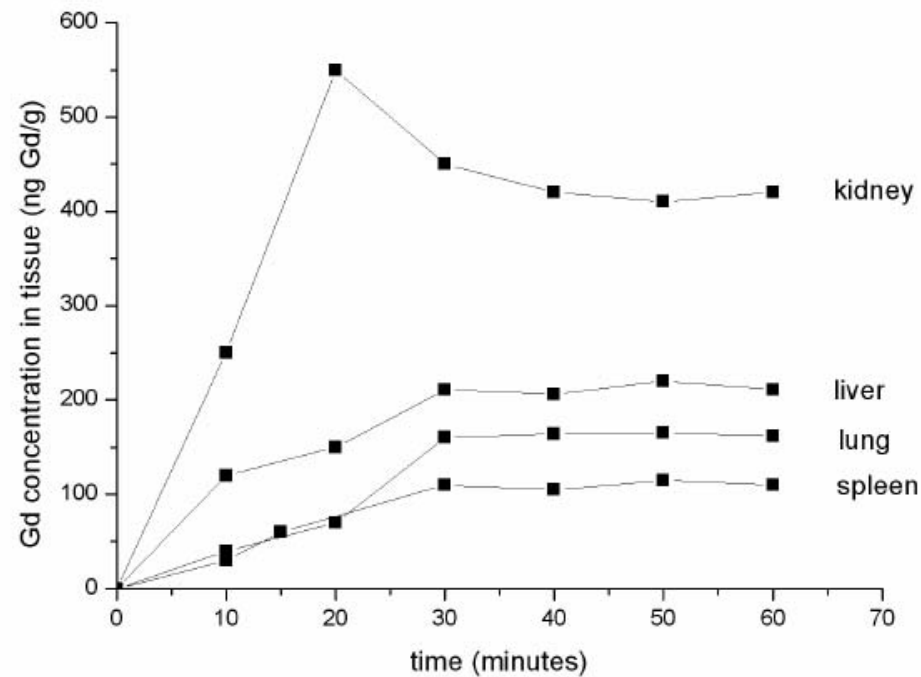


Figure 4. Biodistribution of Gd in kidney, liver, lung, and spleen in mice at different time after administration of Gd@C82(OH)22±2 nanoparticles.

Include important experimental details

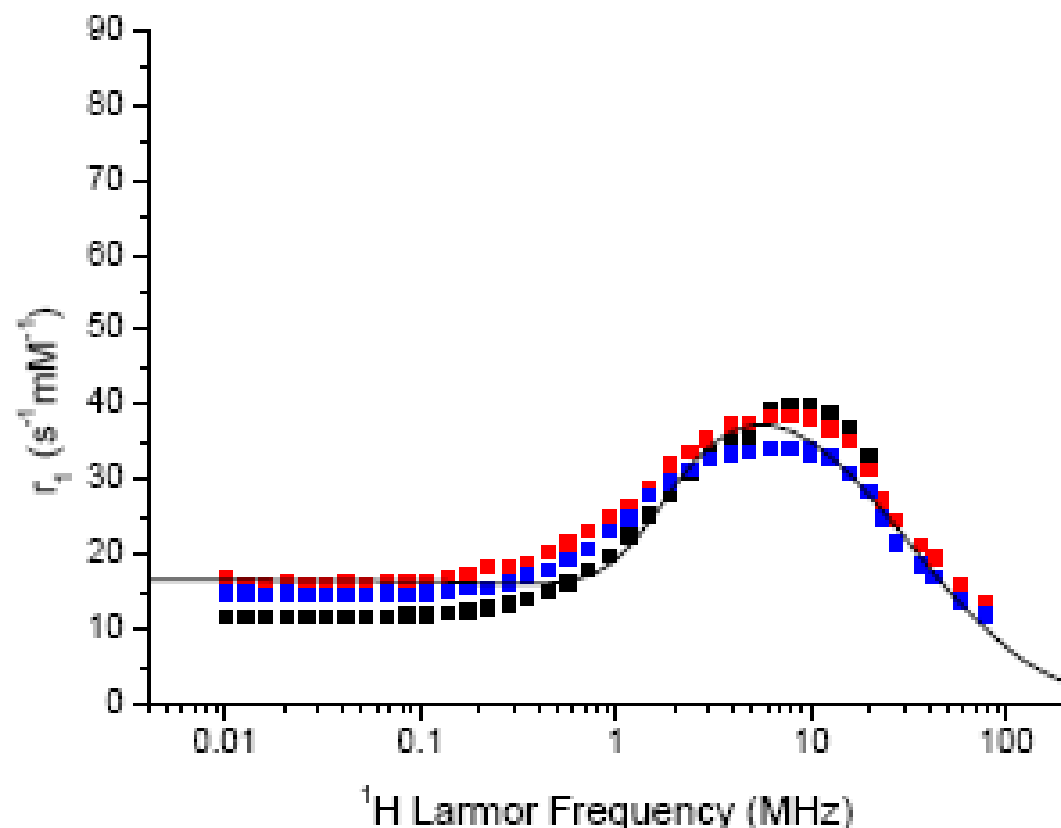


Figure 2. NMRD profiles for the Group I samples A (■), B (■) and C (■). The solid line is a simulation for a SPM dispersion with $D_{\text{core}} = 12$ nm, $\Delta E_{\text{min}} = 1$ GHz, $M_s = 49$ emu.g $^{-1}$. All measurements were carried out at $25^\circ\text{C} \pm 1^\circ\text{C}$, with a measuring frequency of 9.25 MHz, on a Stellar FFC2000.

Identify multiple curves or traces

Can you tell which traces are for the uncrosslinked or Crosslinked SPEEK?

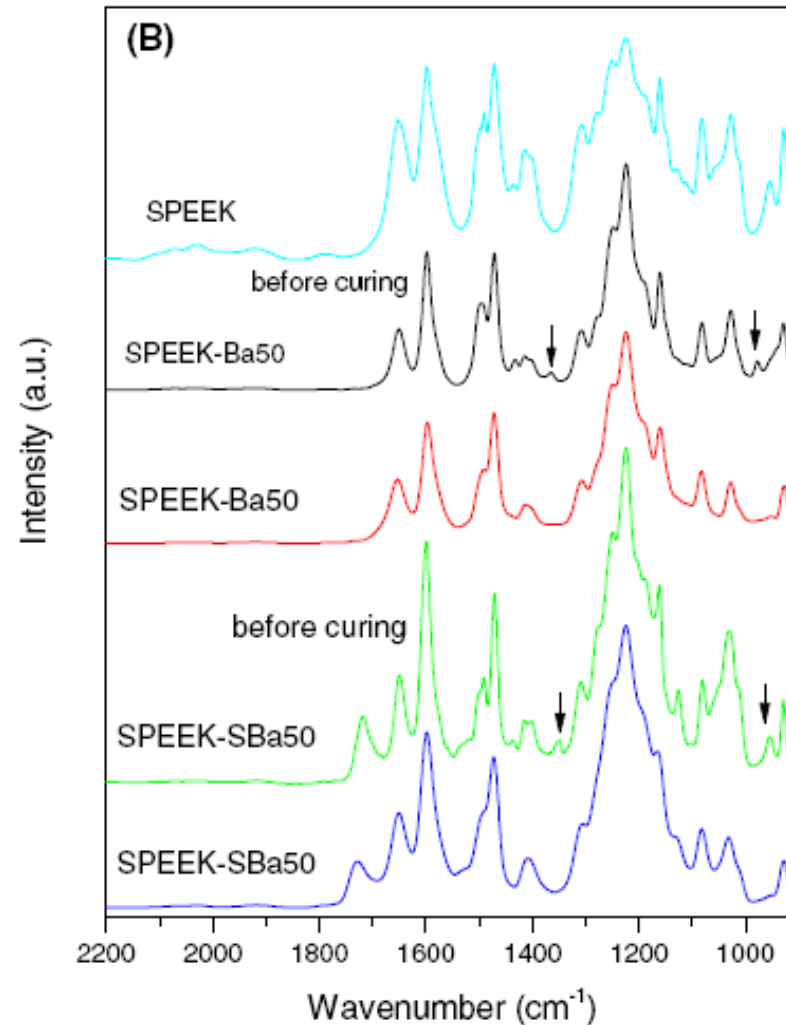


Figure 2. The FTIR spectrum of (A) Ba, ABa and SBa (B) uncrosslinked and crosslinked SPEEK with Ba and SBa membranes, respectively.

Caption should match the graphic

Different symbols in graph and caption

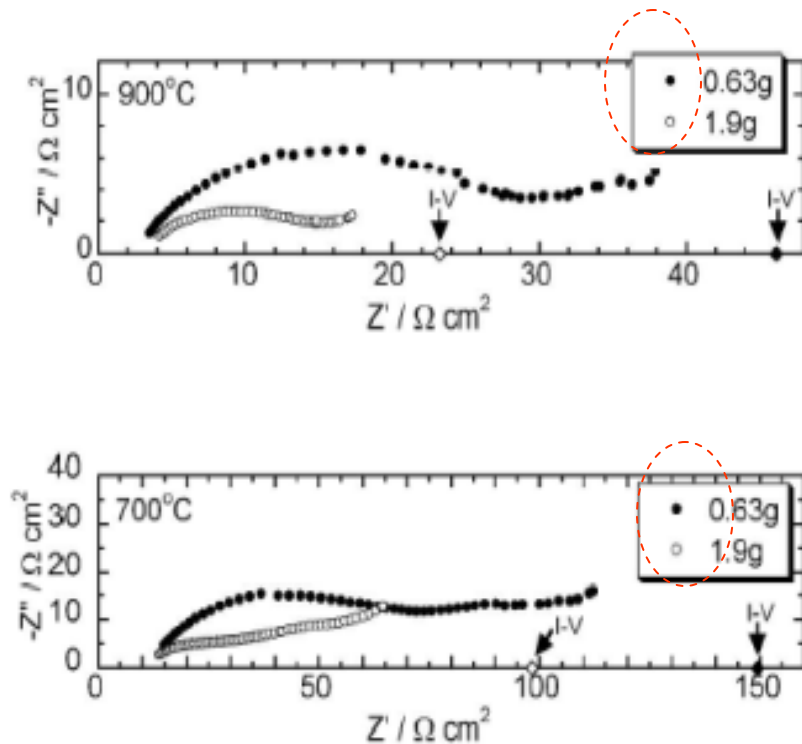


Figure 4. Effect of the amount of the carbon/carbonate slurry on the impedance spectra at 900 and

700°C. (\blacklozenge , \diamond): ASR values at OCV from the I-V curves. Carbon: Super-S.

Caption should match the graphic

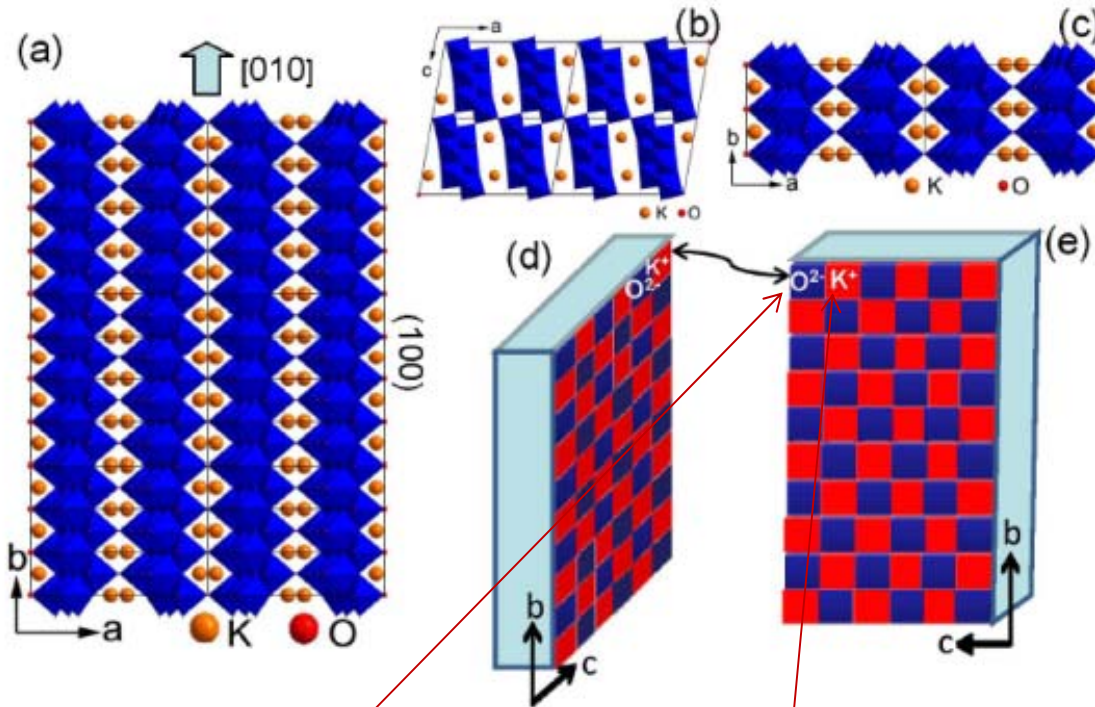


Figure 4. (a) Atomic structure of the $K_2Ti_6O_{13}$ nanobelt, with growth direction $[010]$, side surfaces (100) and top and bottom surfaces (001) . (b) and (c) Projection of the unit cell of $K_2Ti_6O_{13}$ along the b and c axis, respectively. (d) and (e) Schematic chess pattern representation of the cation and anion distribution in the (100) plane, parallel to which the two spiral looks meet. The red area corresponding to O^{2-} , and the blue area corresponding to K^+ .

2. Good Readability

- Good resolution
- Clear, concise, complete
- Font is legible (size, boldness, font choice)
- Colors enhance the graphic not detract
 - Reproducibility (quality doesn't improve upon reproduction)
 - Color blindness and deficiencies
- All parts of figure are identified or explained
- Figure are proofed carefully

Resolution

Can you tell what you are looking at?

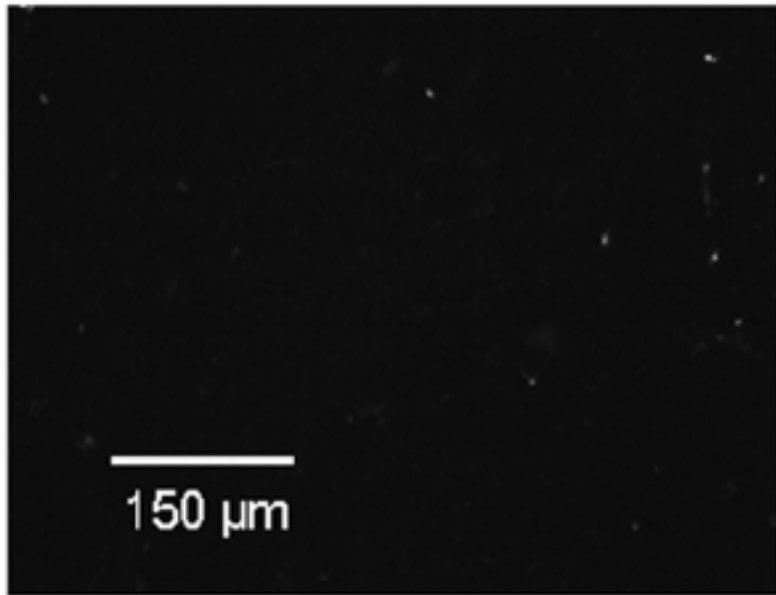
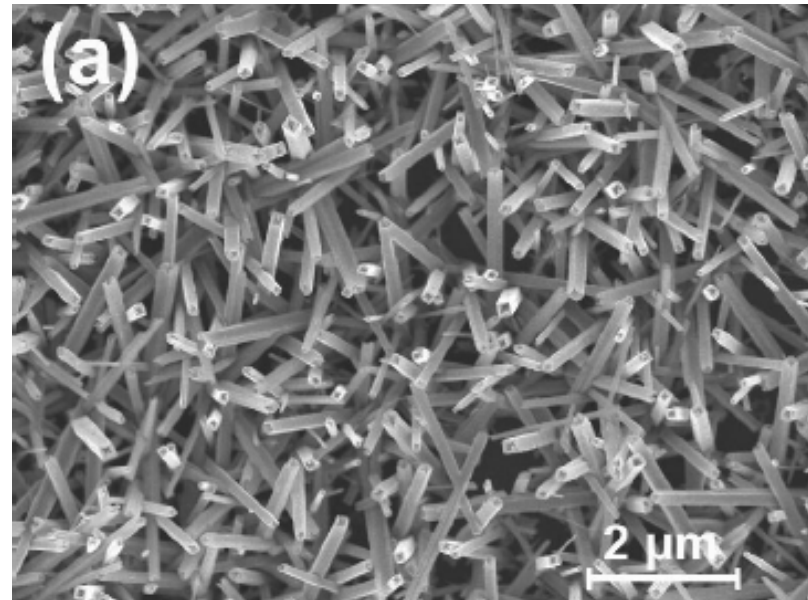


Image is clear



Another example of poor resolution

What can you make out of these AFM figures?

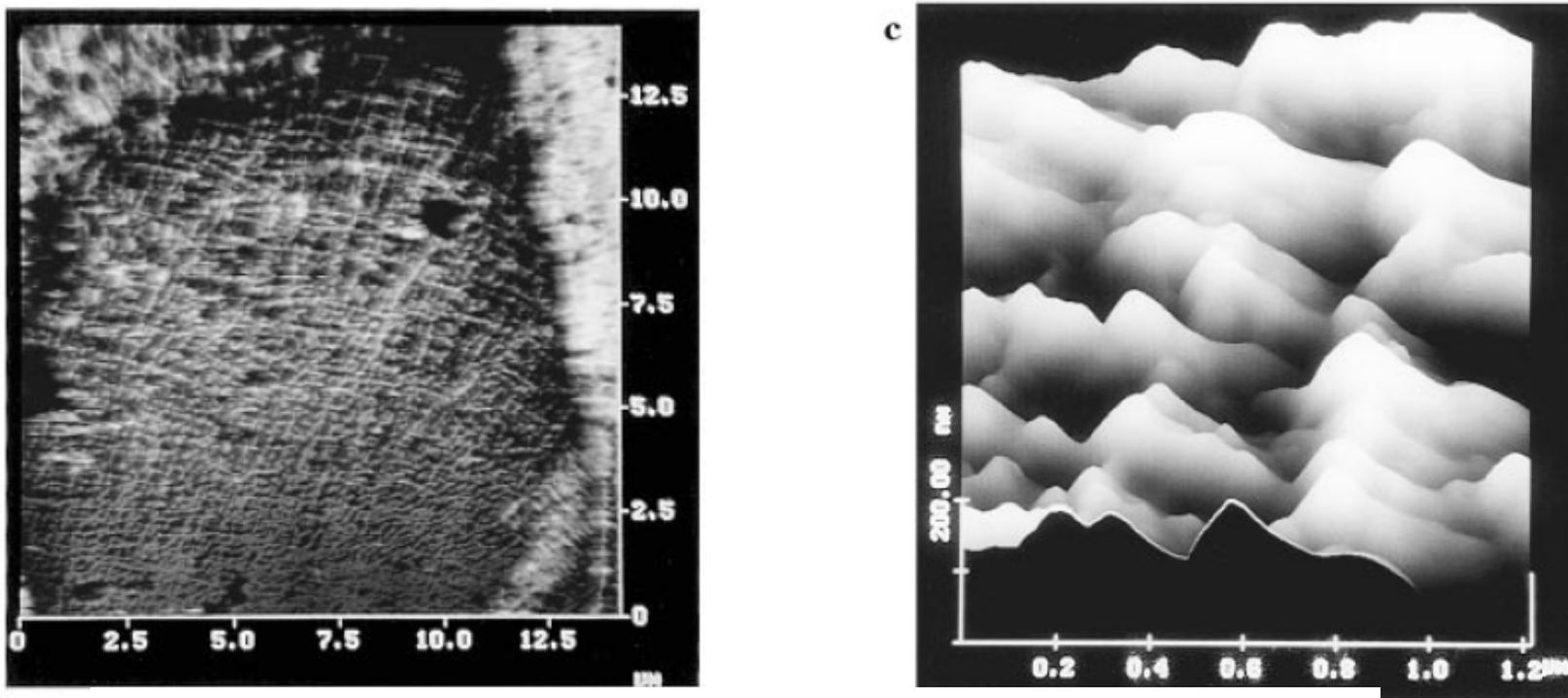
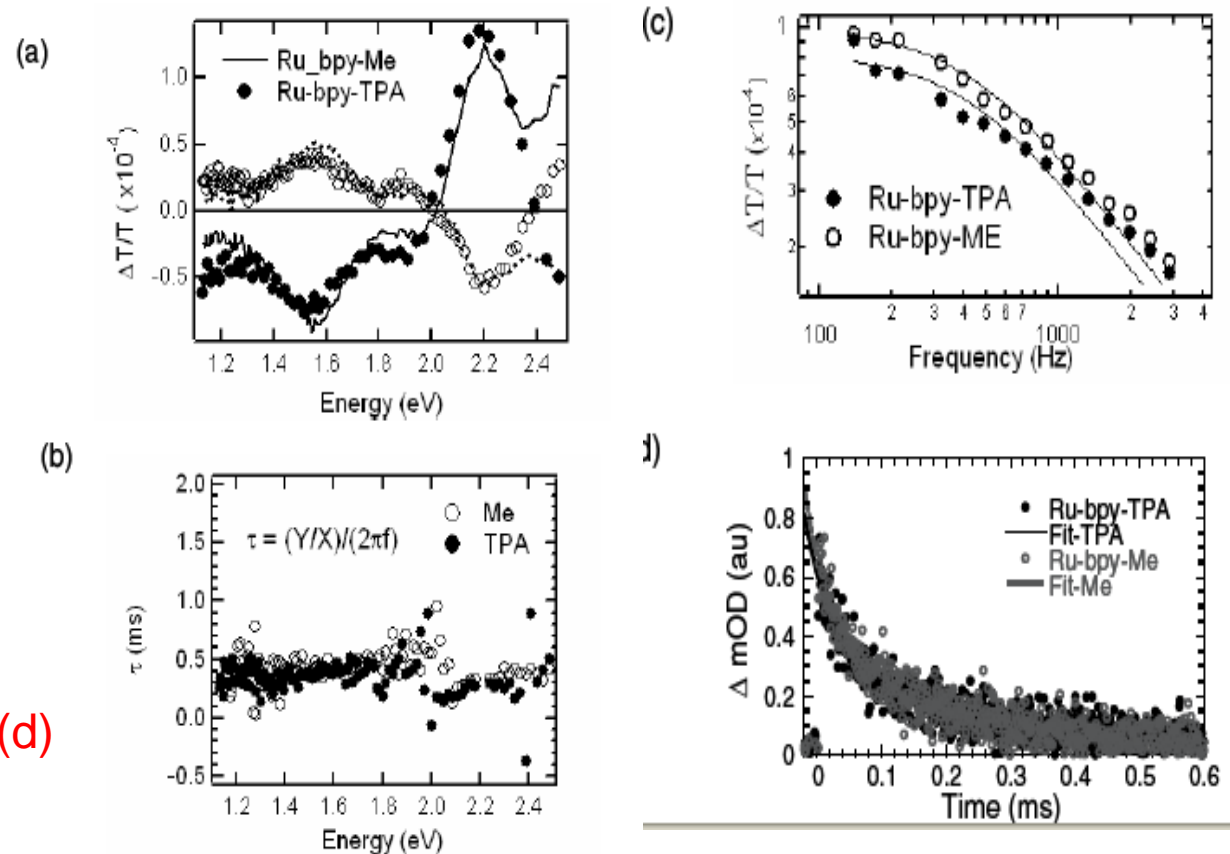


Figure 11. AFM micrograph of a sample isothermally crystallized at 120 °C: (a) an elongated morphology; (b) large-scale image of a network structure of crystalline entities; (c) three-dimensional image of an enlarged area of (b).

Be concise (save ink)

Quickly, can you describe Fig. d?



Where is description for (d)
...or even for (j)

- Figure 2, a) Photo induced absorption (PIA) spectra for 1.4 μm thick mesoporous TiO₂ films sensitized with Ru-bpy-TPA (circles) and Ru-bpy-Me (lines), pumped at 488 nm with an intensity of 128 mWcm⁻² and a frequency of 200 Hz. The open circles and the dashed line correspond to the out-of-phase signals for the Ru-bpy-TPA and Ru-bpy-Me respectively. b) The frequency dependence of the PIA signal ($\text{dr} = (\text{dx}^2 + \text{dy}^2)$) at 800 nm (1.55 eV) under the same pump beam conditions as above. c) Transient absorption spectroscopy (TAS) of two similar samples to above, Ru-bpy-TPA (dark solid circles, solid line) and Ru-bpy-TPA (gray open circles, dashed line) of the transient absorption signal at 650 nm (~ 1.9 eV absorption of the oxidized dye species). The pump was at 600nm with a pulse width of ~ 5 ns with 35 $\mu\text{J}/\text{pulse}$ and a repetition rate of 30 Hz.

Be concise (ex. 3)

Can you distinguish these curves?

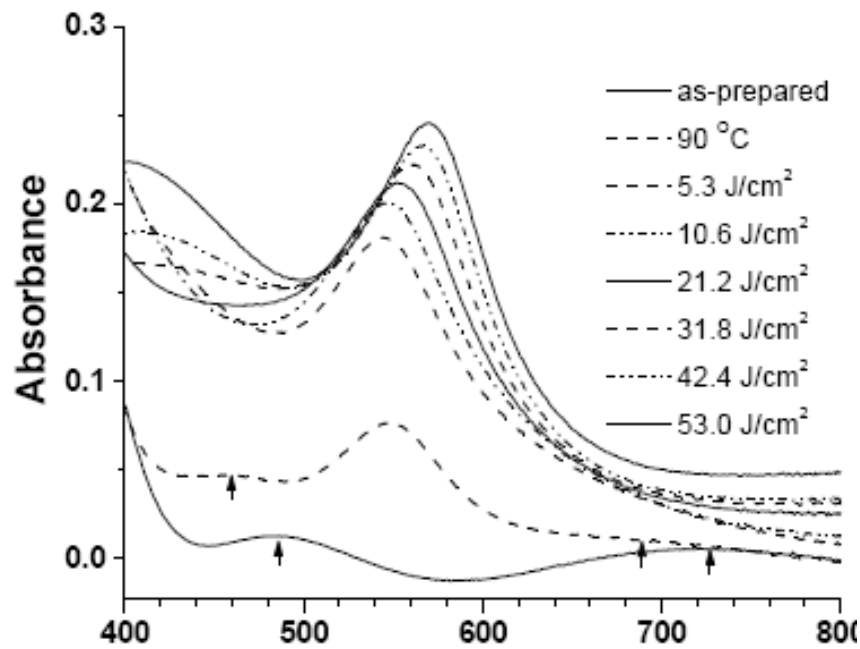
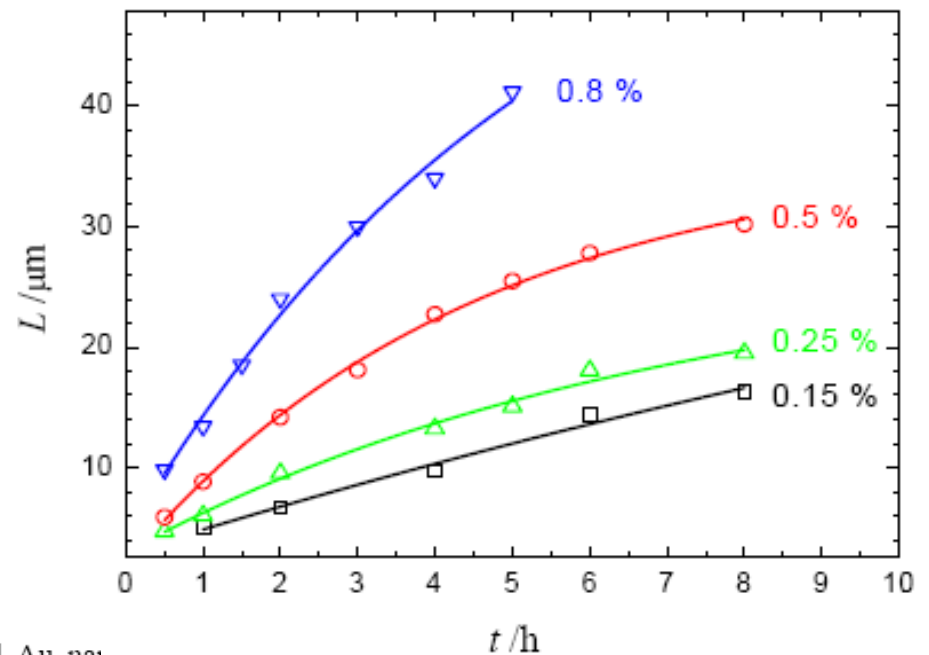


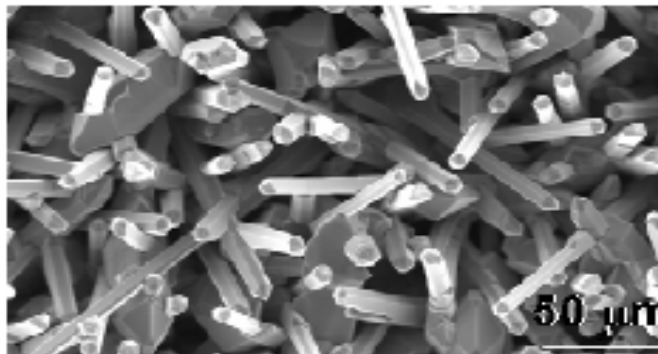
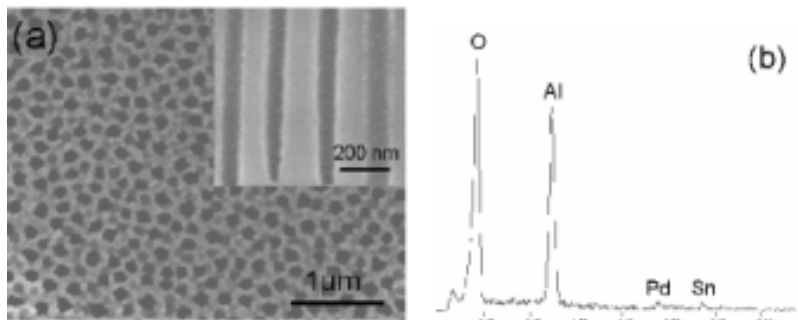
Figure 3 Optical absorption spectral evolutions of in-situ generated Au nanoparticles inside the hybrid (SiO₂-TiO₂-PEO) film matrix with respect to the thermal-treatment energies.

Clear, concise, easy to read



Legible Font Size

Font too small



Adequate font size

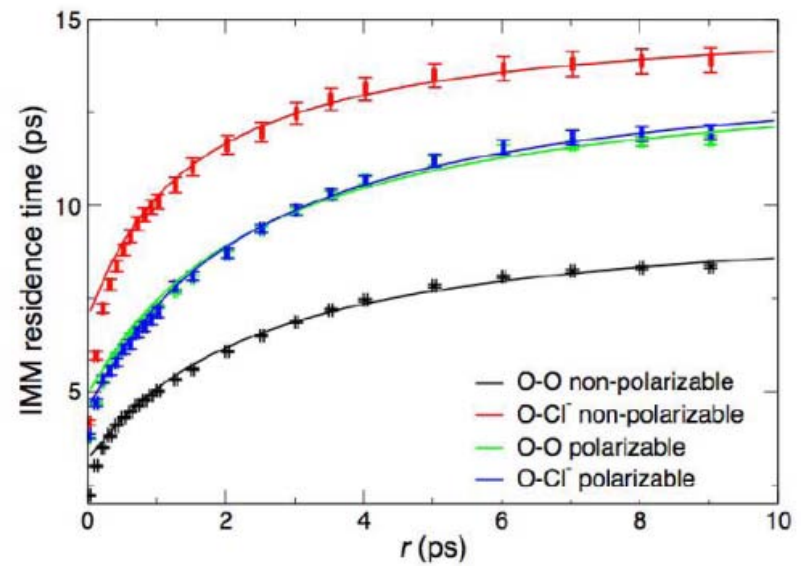
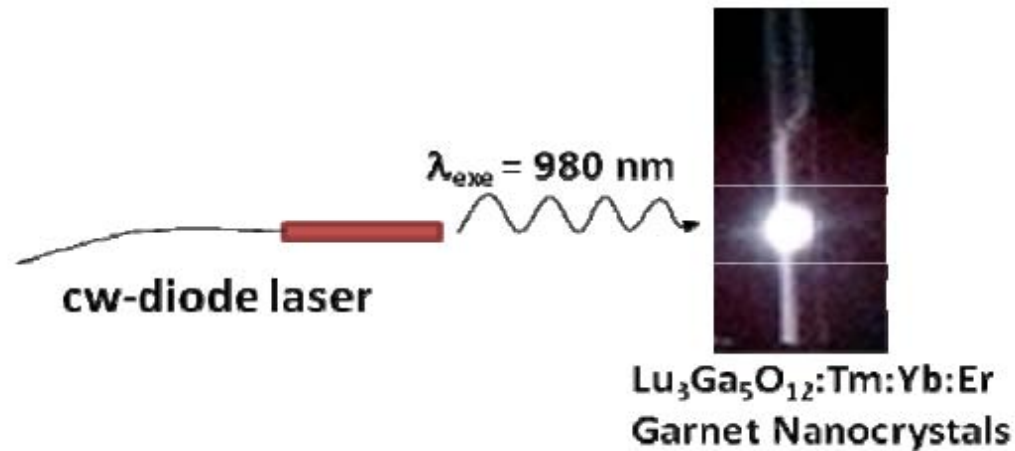


Figure 1

Legible Font – Avoid bolding the entire graphic

Bolding all characters often makes it more difficult to read.
Use bolding only for **emphasis**.

TOC figure



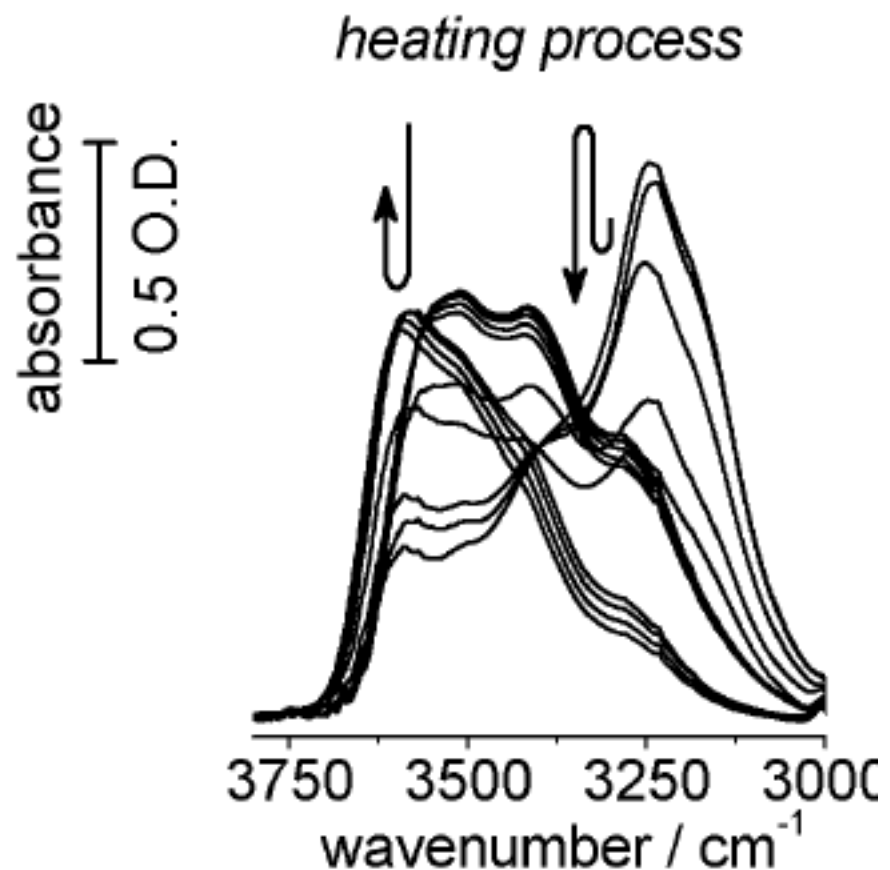
Legible Fonts

- Use bolding selectively
- Use large font size
- Use both upper and lower case letters
- Use serif font

Color can enhance a graphic

Can you distinguish the individual spectra?

Proper use of color would have improved the readability.



Color can enhance a graphic

Hard to distinguish multiple data series in B&W

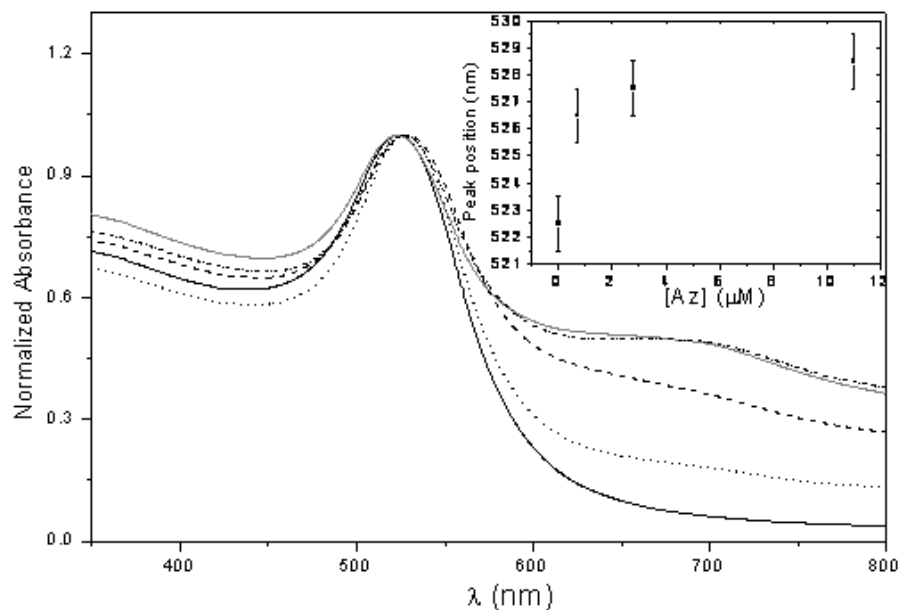
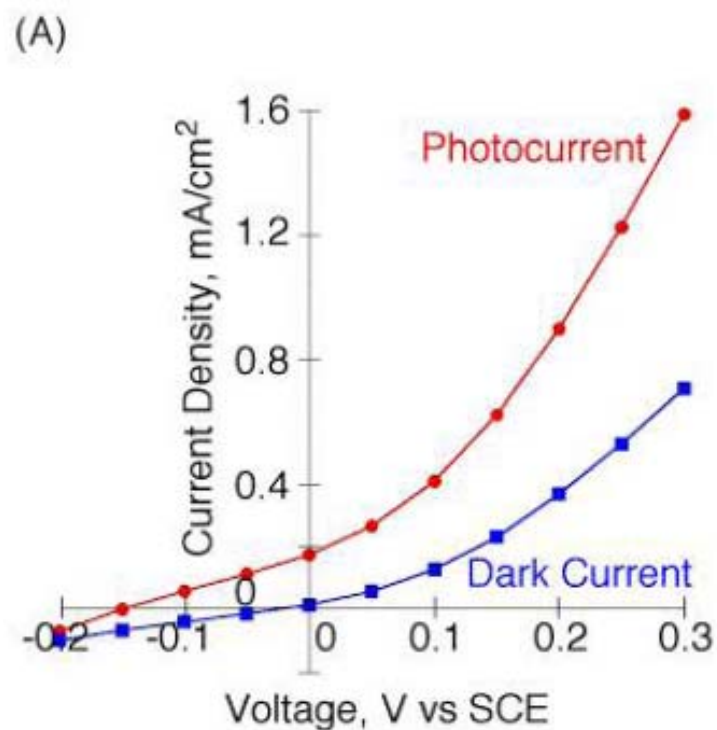


Figure 2. Normalized absorption spectra of commercial AuNP solution ($[\text{AuNP}] = 1.13 \text{ nM}$) (continuous black line) and of Az+AuNP solutions at $[\text{AuNP}] = 1.02 \text{ nM}$ and various Az concentrations: 0 μM (continuous gray line), 0.7 μM (dash-dotted black line), 2.8 μM (dotted black line), 11 μM (dashed black line). Inset: Plasmon peak position dependence on Az concentration as obtained by multi-peak Gaussian fitting procedure.

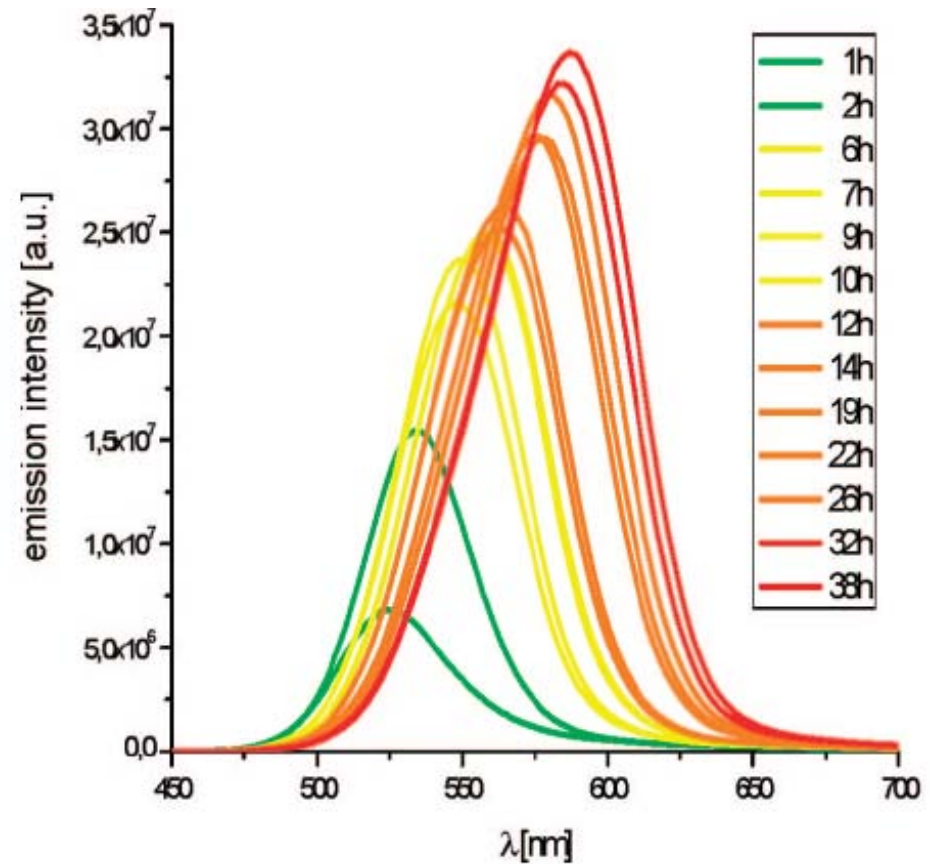
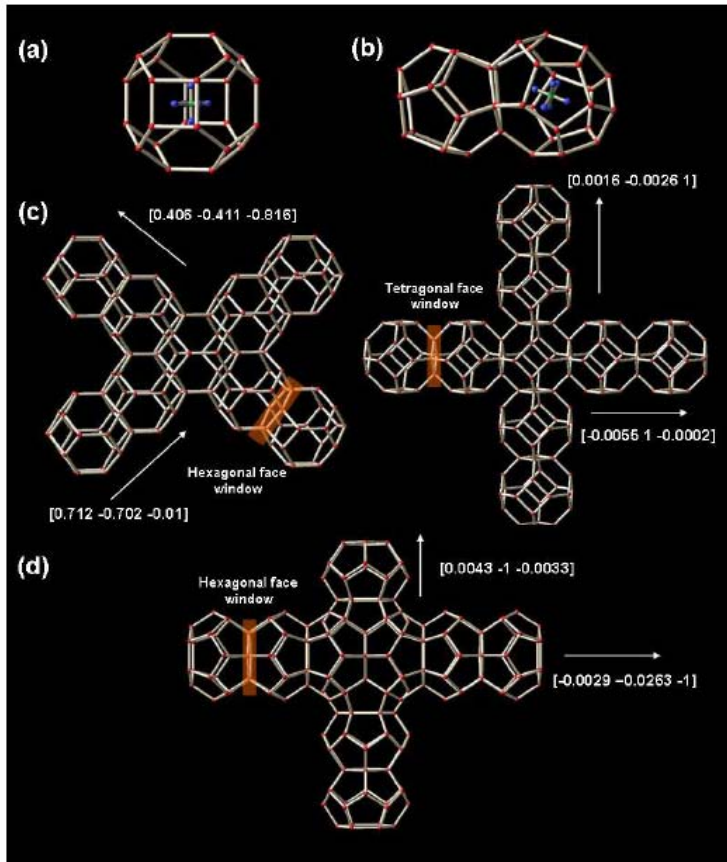
Use of color, different data point symbols greatly improves readability



Avoid colors that don't reproduce well

Dark backgrounds

Yellow (or other light colors)



Avoid colors that are difficult to distinguish

Similar looking colors

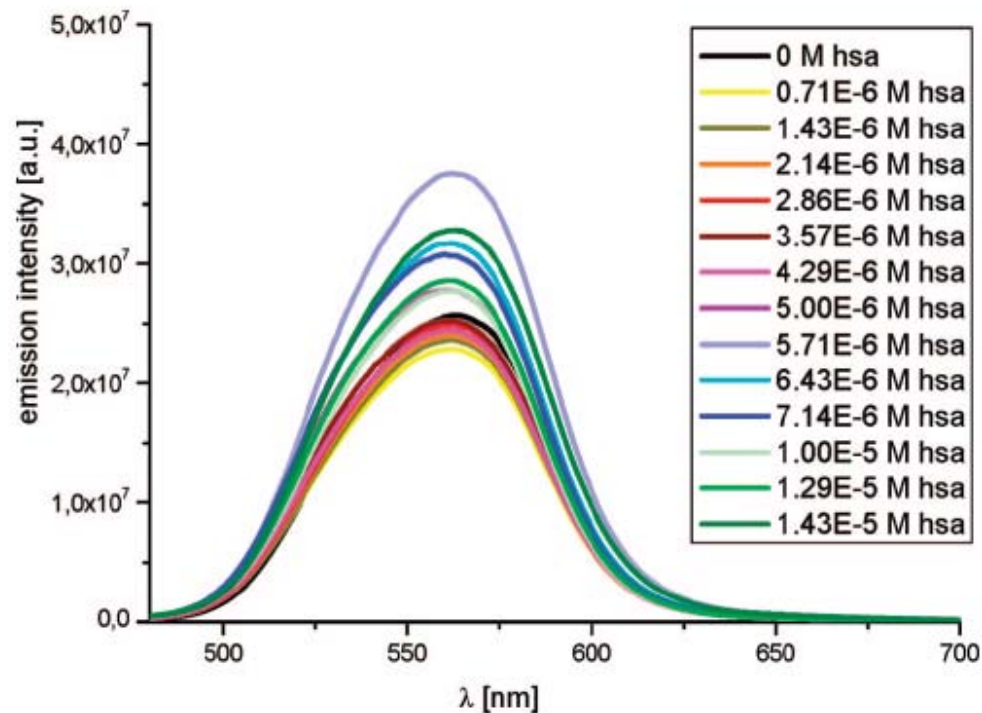
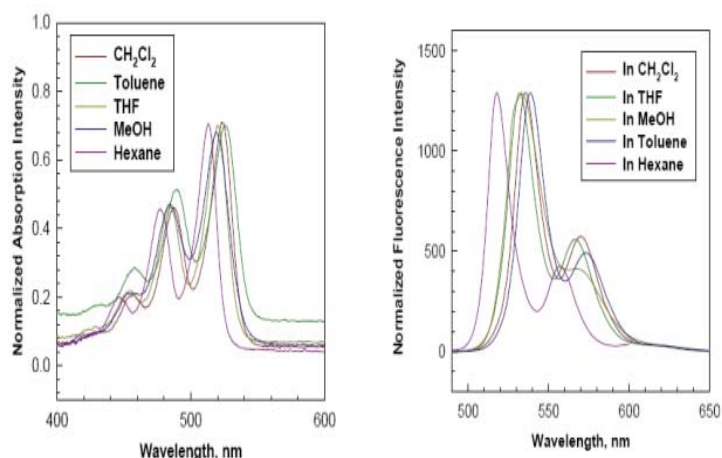


Figure 10. Emission spectra (excited at 300 nm) of N3 (5 ± 10^{-5} M) in water in the presence of different concentrations of human serum albumin (0 to 1.43 ± 10^{-5} M). Please notice the continuous increase of the emission intensity.

Consider readers with color blindness or deficiencies

Would a color blind/deficient person be able to distinguish these curves?

In a B&W printout, could you distinguish the different traces?



1a

1b

Figure 1. UV-vis and fluorescence spectra of DIE1 at 20 °C in hexane, toluene, CH₂Cl₂, MeOH, THF (1 × 10⁻⁶ M). Both the absorption and fluorescence spectra were normalized at the 0-0 transition maximum.

transition maximum.

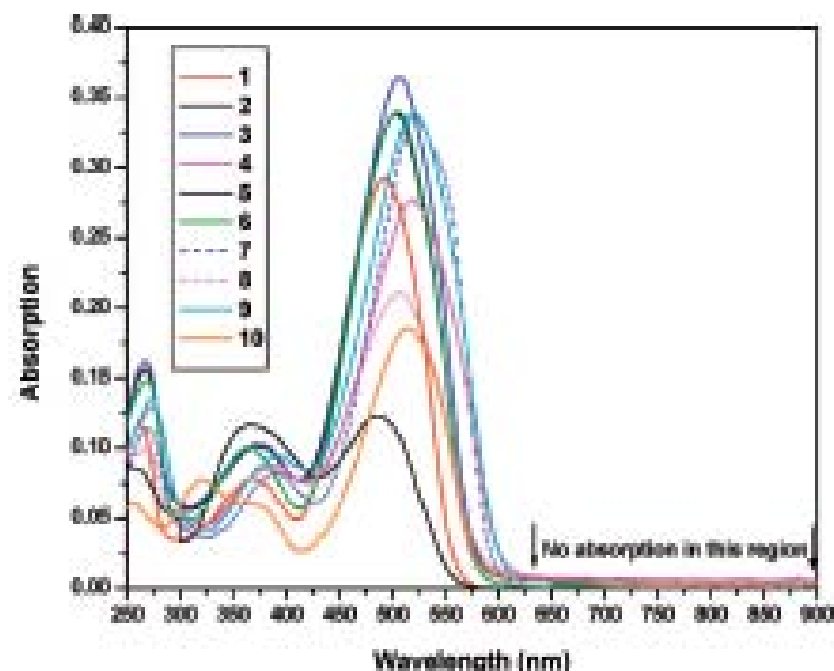


Figure 5. UV-vis absorption spectra of Croconate dyes 1–10 in CHCl₃.

Help readers with color blindness or deficiencies

Identify individual traces with tags (a,b,c...)

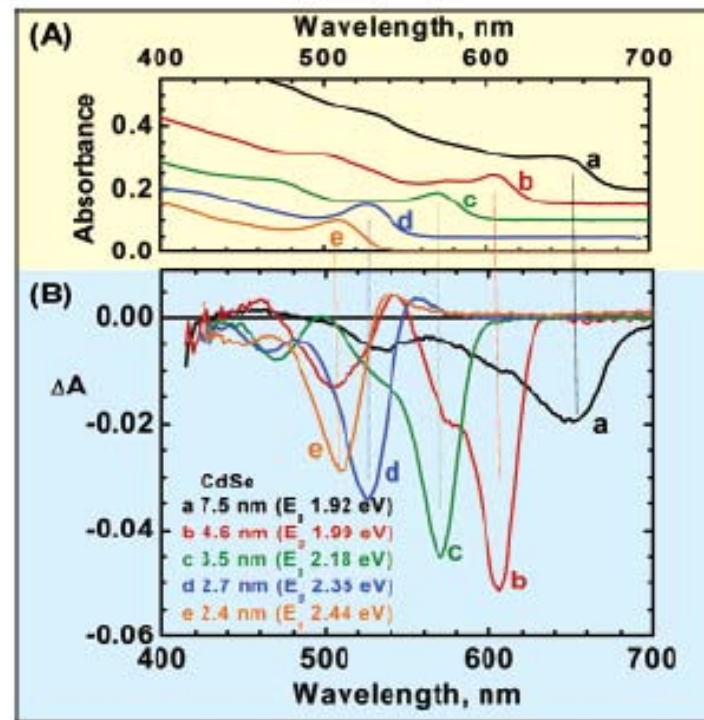
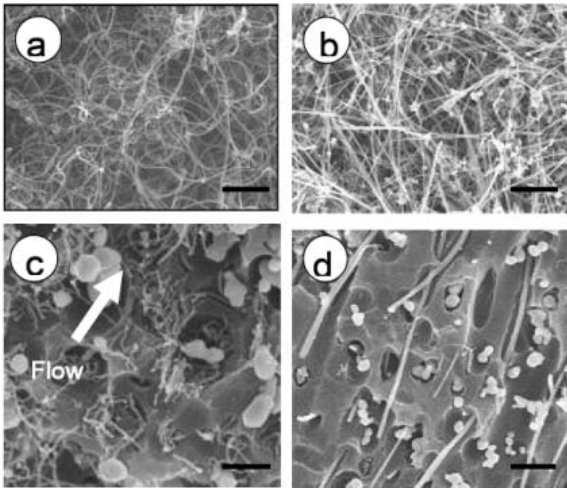
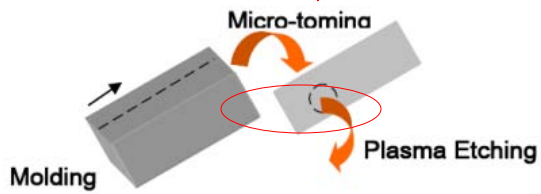


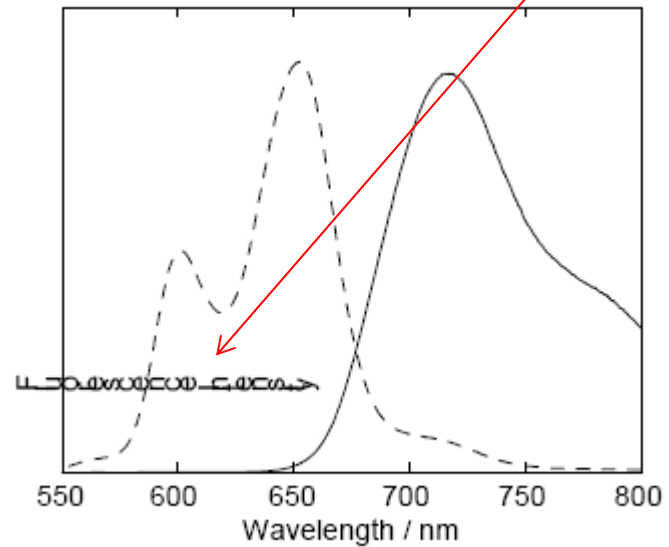
Figure 1. (A) Absorbance spectra of CdSe quantum dots in toluene. (Y-axis offset is introduced for clarity.) (B) Transient absorption spectra recorded 2 ps following the 387 nm laser pulse excitation of different size CdSe quantum dots in 1:1 ethanol/tetrahydrofuran (THF).

Proof the final version carefully

Part of text hidden



Axis label has rotated 90°

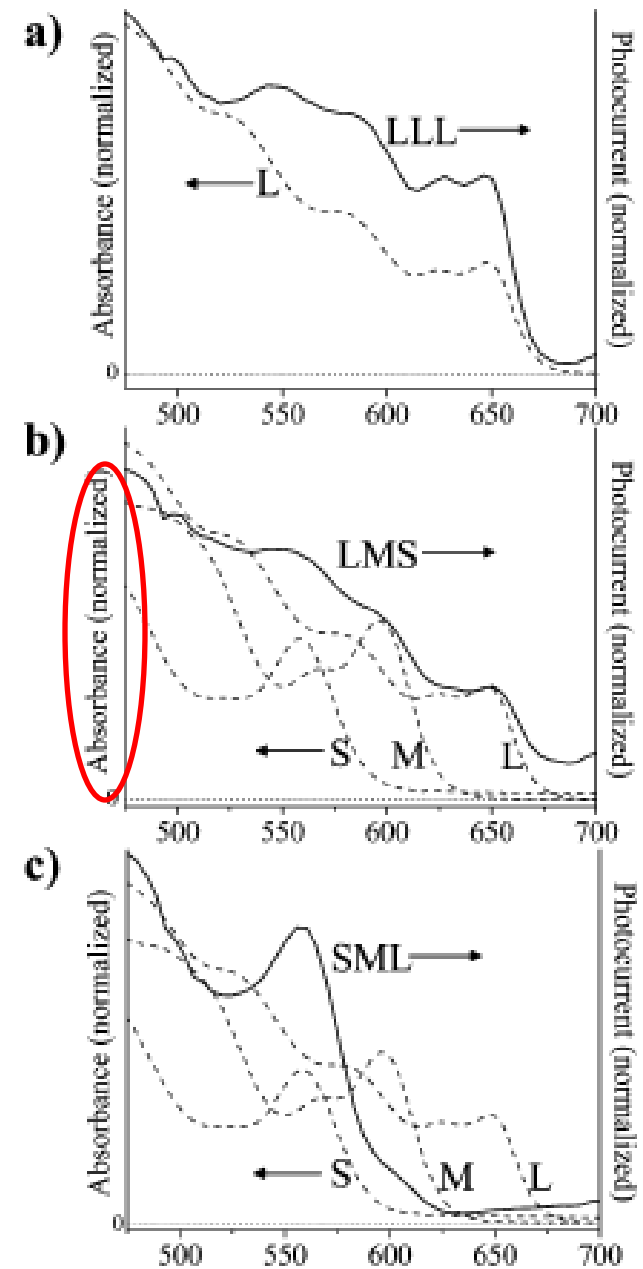


Watch for formatting changes

All parts of figure should be identified or explained

To what are these normalized?

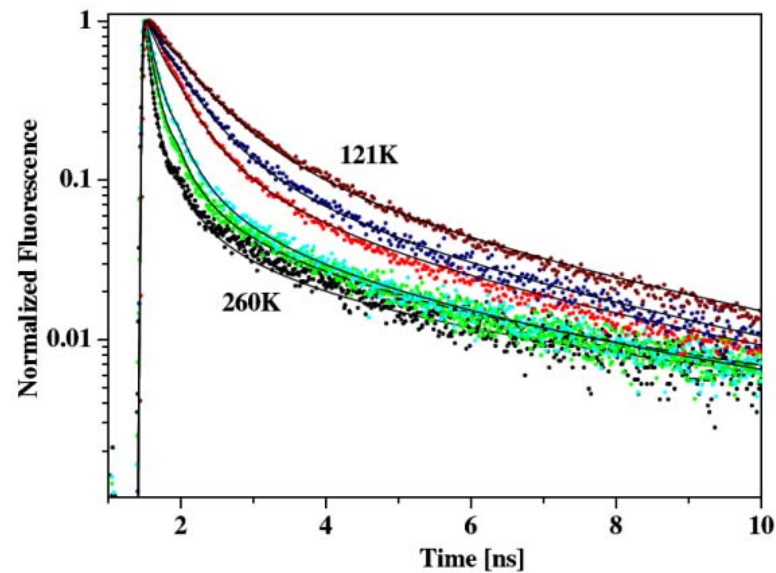
Figure 6. Photocurrent action (PCA) spectra (normalized photocurrent as a function of excitation wavelength, solid lines, right axes) for the junctions ITO/PEDOT:PSS/X/EGaIn, X = LLL (a), LMS (b), and SML (c). The tunable excitation source for these spectra was a 450 W Hg–Xe arc lamp in combination with a monochromator (intensity = $38 \mu\text{W}/\text{cm}^2$). Also shown with each PCA spectrum are the ground-state absorbance spectra for films of the S, M, and L QDs on glass (dashed lines, left axes).



No axis title

Unidentified Features (ex. 2)

What is the significance of colors?



Note: 80-280K in caption

Fig 5

Figure 5 - Model fitting (solid line) of the experimental time-resolved emission data (dots) of G4 wires at several temperatures in the range of 80-280 K.

Unidentified Features (ex. 3)

Which is a? b?

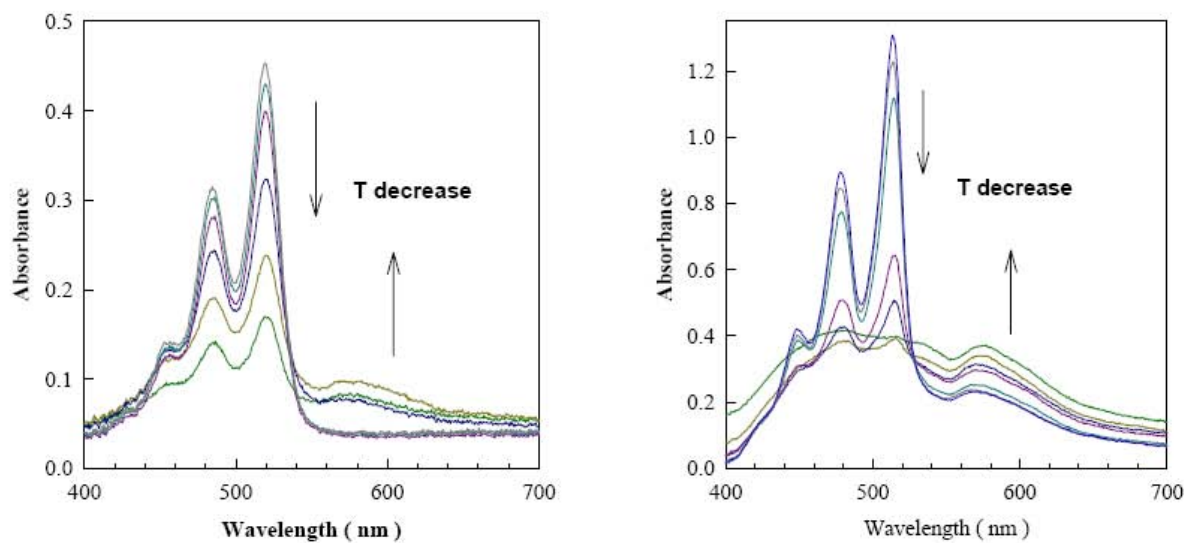


Figure 3. Temperature-dependent UV-Vis adsorption spectra of **D1E1** (1×10^{-5} M) in a) methanol, b) methylcyclohexane. Temperature between 20 and 70 °C at 10 degree increments.

Unidentified Features (ex. 4)

Don't forget to check the footnotes

Table 2 Effects of annealing in N₂ on the dispersion, cluster size, activity and selectivity of RuO₂(9.5wt%)/CNT catalyst.

Annealing temperature °C	d_{RuO_2} ^b nm	Dispersion ^c %	Conversion rate ^a mol _{MeOH} (mol Ru _{total}) ⁻¹ h ⁻¹	Turnover rate ^d mol _{ODH} (mol Ru _{surface}) ⁻¹ h ⁻¹	E_{ODH}^{obs} ^e kJ/mol	S _{CO2} %	S _{FA} %	S _{MF} %	S _{DMM} %
100	1.4±0.5	39.8	158	232	48.0±0.9	0	17	34	49
200	1.5±0.5	41.5	100	147	-	0	22	41	37
300	1.6±0.4	45.4	124	171	60.9±3.7	0	25	52	22
400	1.5±0.5	35.7	79	141	-	0	27	66	6

a Reaction conditions: 120 °C, 7 kPa methanol, 20 kPa O₂, conversion in 13~25%.

b By TEM.

c By CO chemisorption.

d The formation of every molecular of MF and DMM need a single ODH event.

?

Unidentified Features (ex. 5)

What are A, B, C?

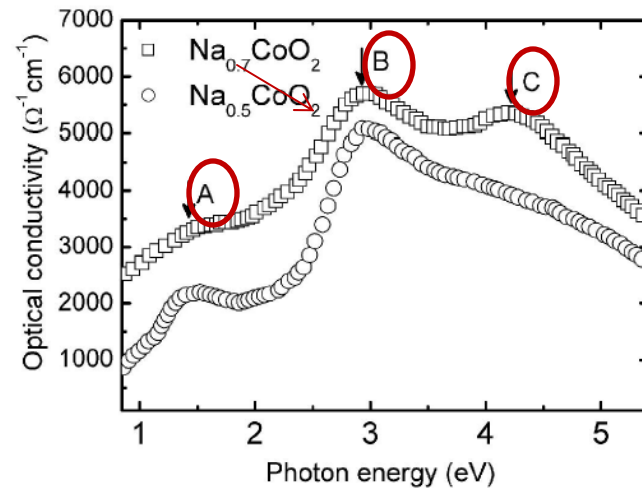


Figure 4

Optical conductivities of $\text{Na}_{0.5}\text{CoO}_2$ and $\text{Na}_{0.7}\text{CoO}_2$ thin films.
98x82mm (600 x 600 DPI)

Unidentified Features (ex. 6)

What is the red line?

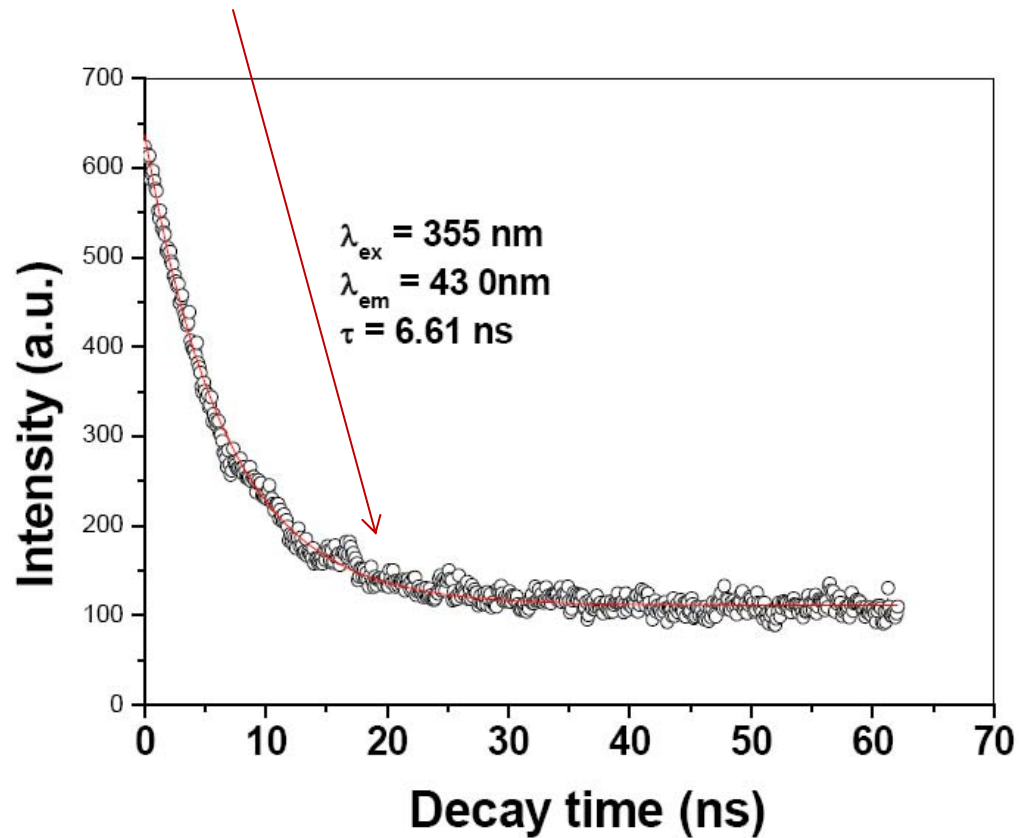


Figure 5 Decay curves of YOSG550 sample.

Unidentified Features (ex. 7)

What are these points? (Don't forget to identify the insets.)

What unit of concentration?

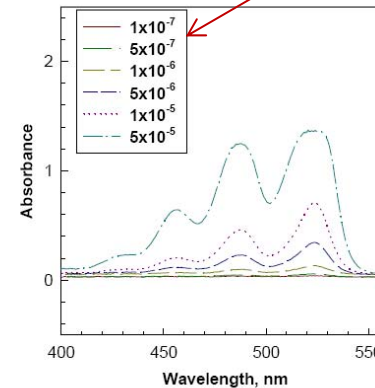
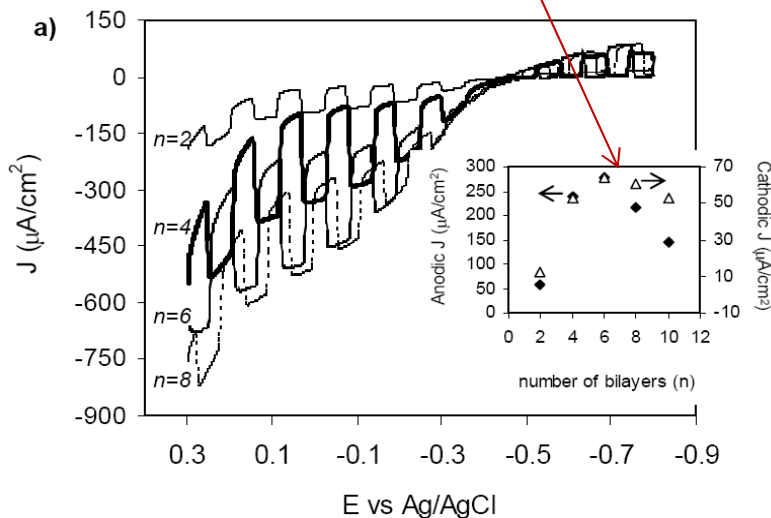


Figure 2. UV-Vis of D1E1 at 20 °C in CH_2Cl_2 at various concentrations.

Figure 4. I-V plots under *chopped-illumination* at (PDDA/Q-CdS)_n bilayers by dip-spin SA

with $n = 2, 4, 6, 8$ in deoxygenated 0.1 M Na₂S/0.2 M NaOH at 20 mV/s (a), anodic and cathodic photocurrents vs. n measured from I-V plots at 75-110 mV, and -630--665 mV, respectively (inset of a), and photocurrent action spectra (% IPCE vs. wavelength) at bilayers $n = 2, 4, 6$ in the same electrolyte (b).

3. Label Axes Clearly

Axis not labeled

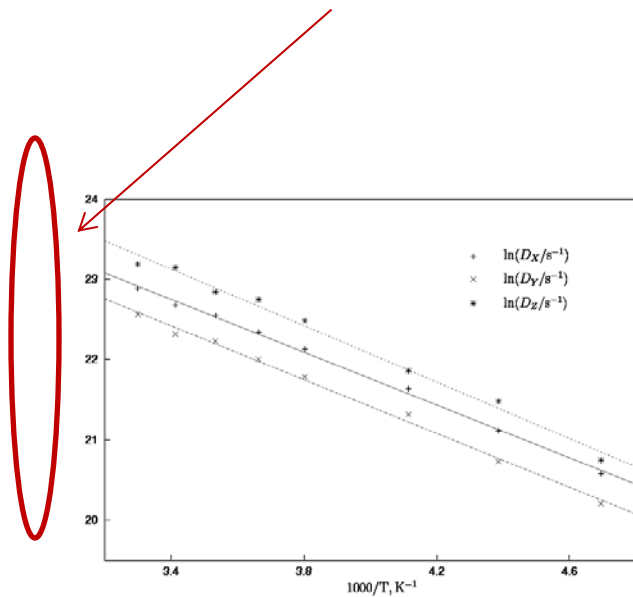
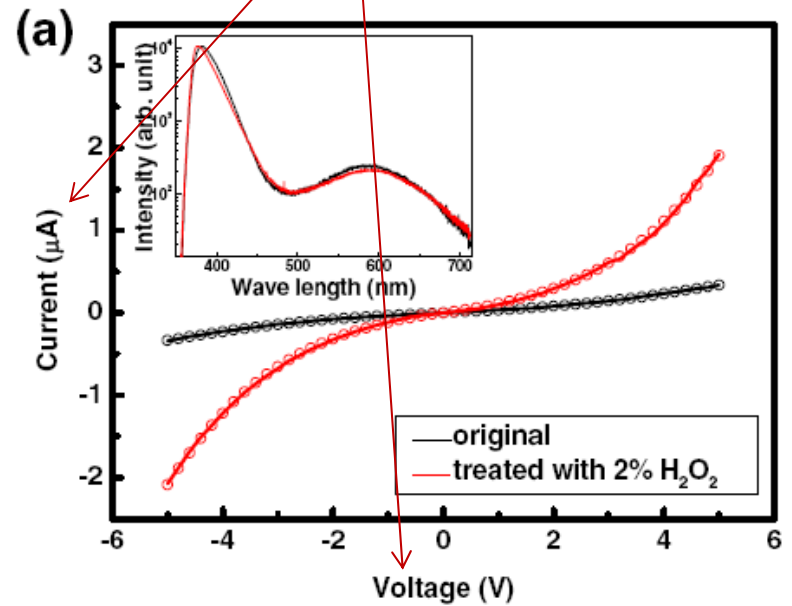


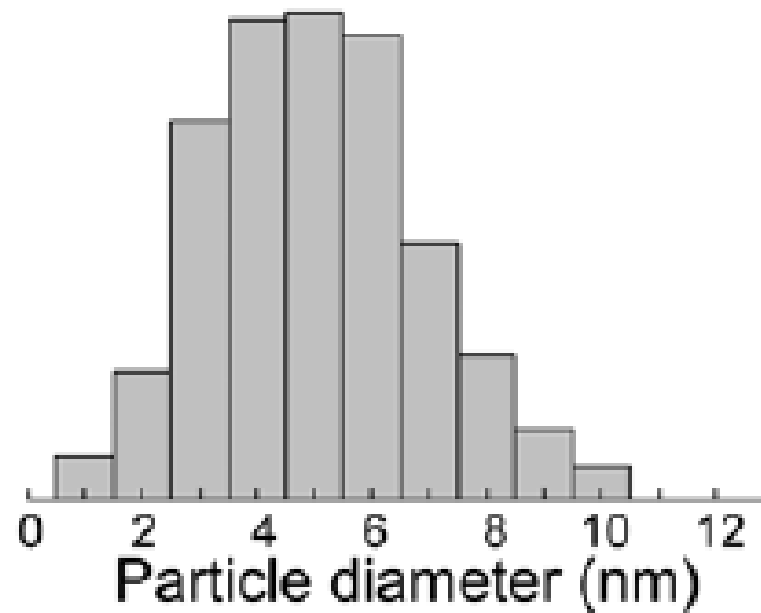
Figure 2: Arrhenius plot for components of the RDT of DMAN. The activation energies extracted from the slopes of these lines are 13.7 ± 0.3 , 13.9 ± 0.4 and 14.6 ± 0.6 kJ/mol for tumbling about X, Y and Z axes, respectively.

Axes clearly labeled



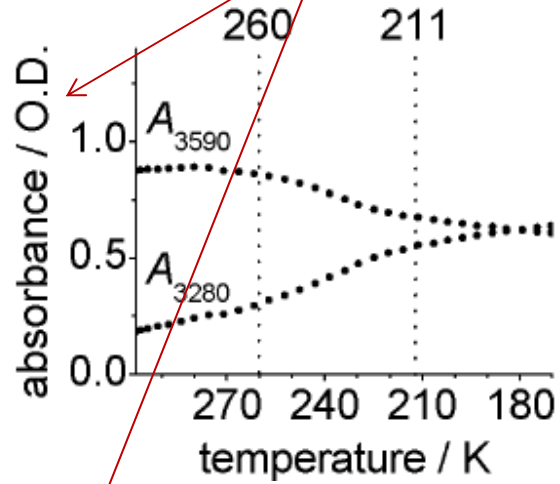
Include a y-axis

y-axis is missing



Use the *Correct* Unit

Wrong Units on Y axis



Correct Y axis

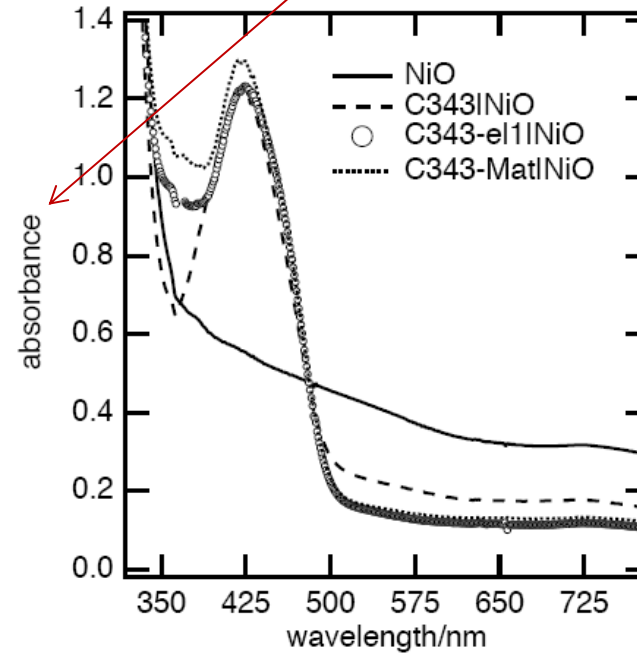
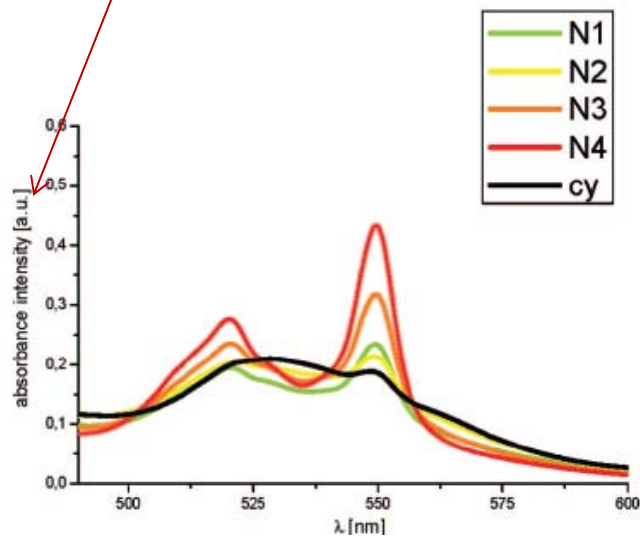
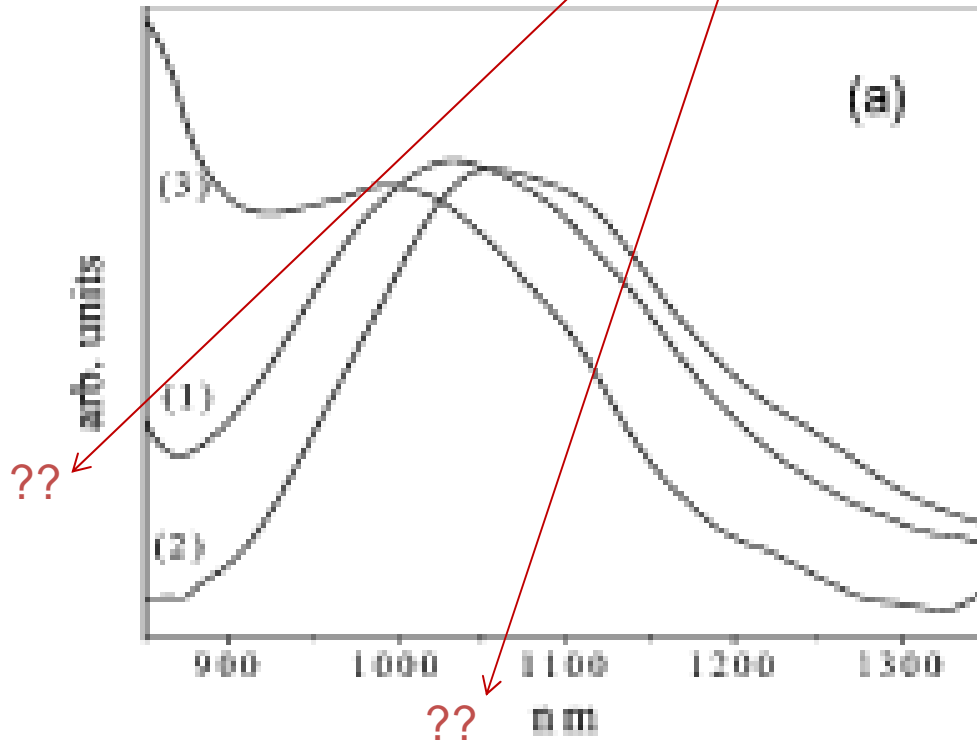


Figure 2:



Identify the Variable



Use the *Correct (!)* Variable

The X-axis should be time

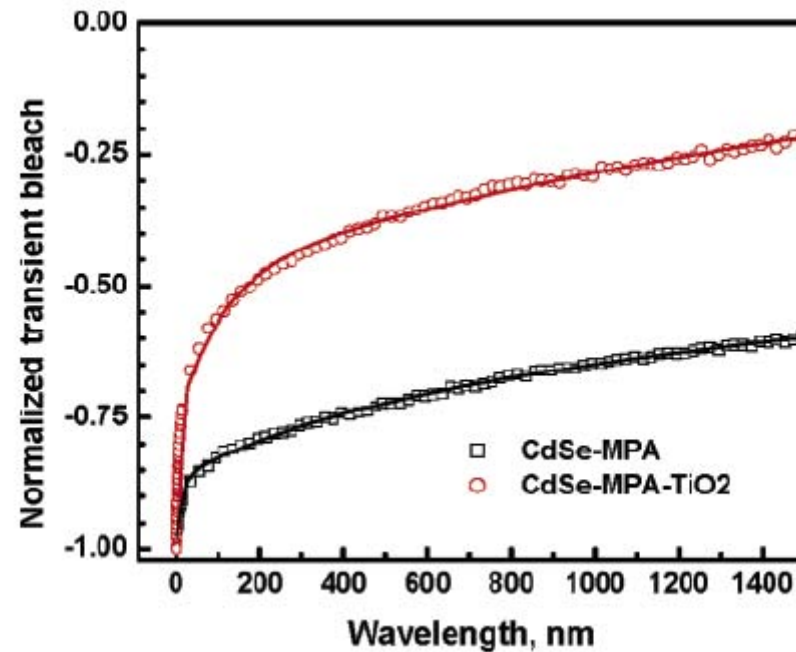
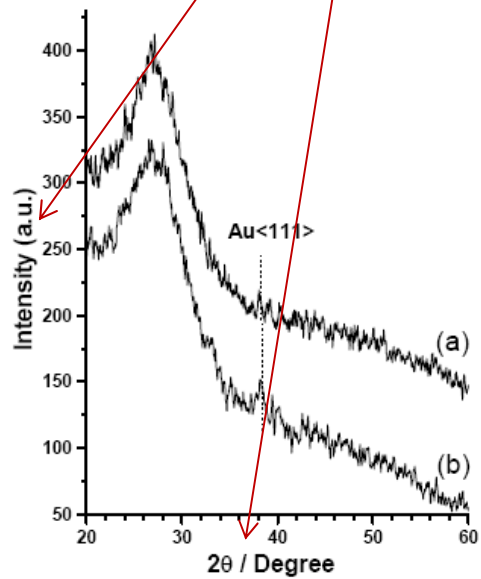


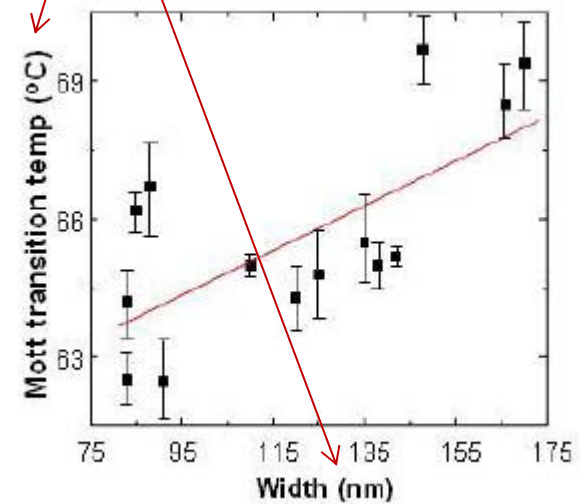
Figure 6. Long time-scale absorption recovery profiles at 530 nm recorded following the 387 nm laser pulse excitation of CdSe-MPA and CdSe-MPA-TiO₂.

Use the same format

Different formats



Consistent format



Avoid only symbols with less common variables

No description

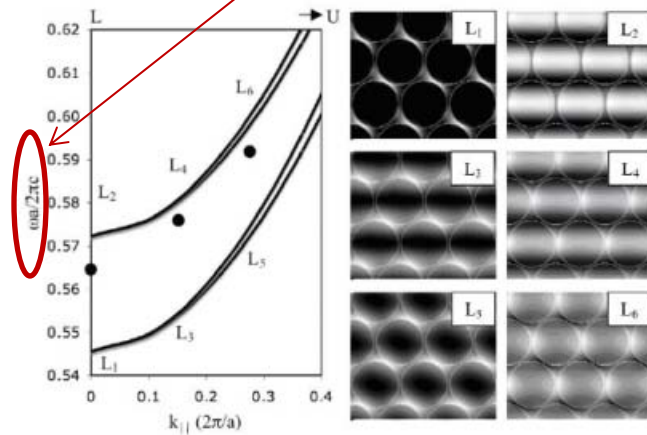
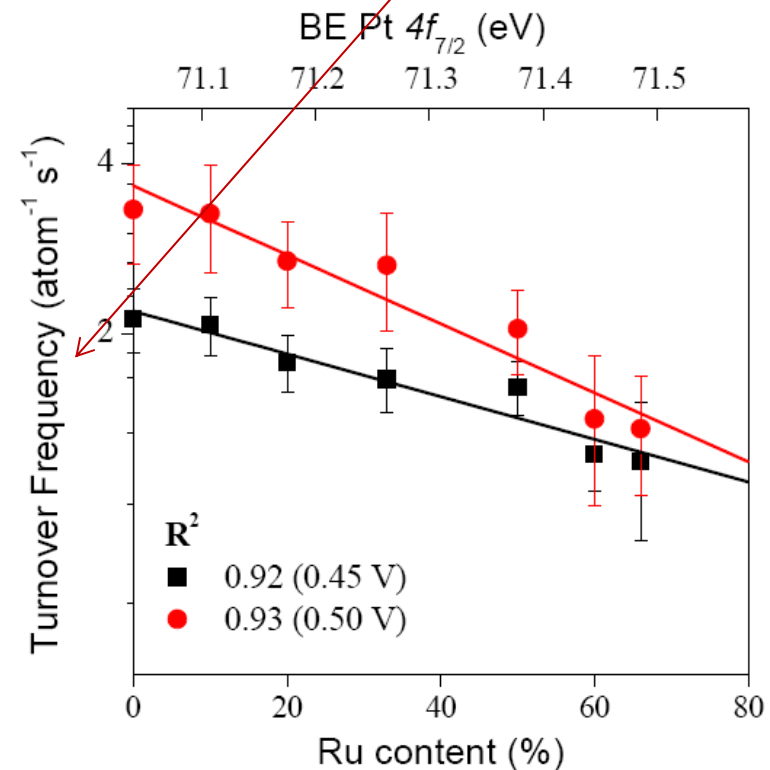


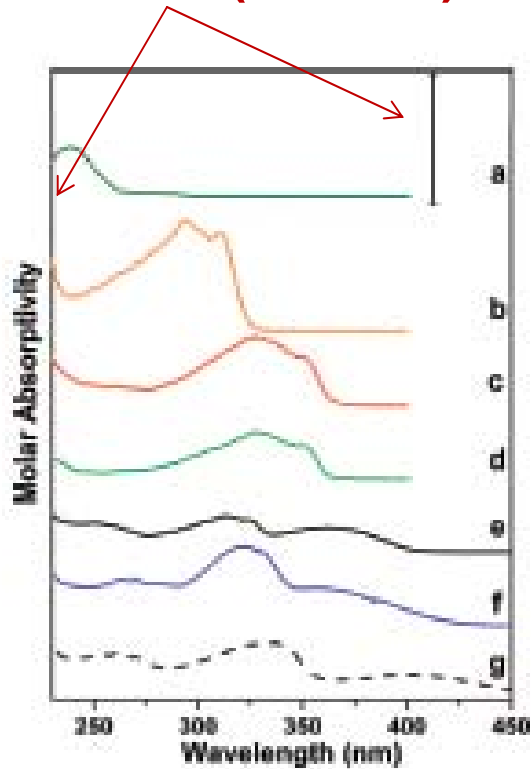
Figure 5. Left panel: Photonic Band diagram of a TiO_2 PC in LU direction. The black dots indicate the transmission dips (0° , 15° and 30°) in the angle-resolved transmission measurement (from Fig. 2). Right panel: The intensity plot $|E|^2$ of modes L_1 & L_2 (0°), L_3 & L_4 (15°) and L_5 & L_6 (30°). White indicates high intensity.

Variable is described



4. Include a Scale or Scale Bar (if appropriate)

No scale (or units) on y-axis



Scale provided

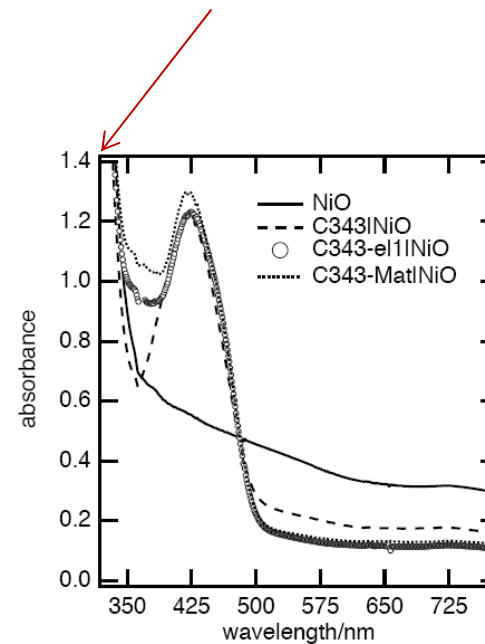
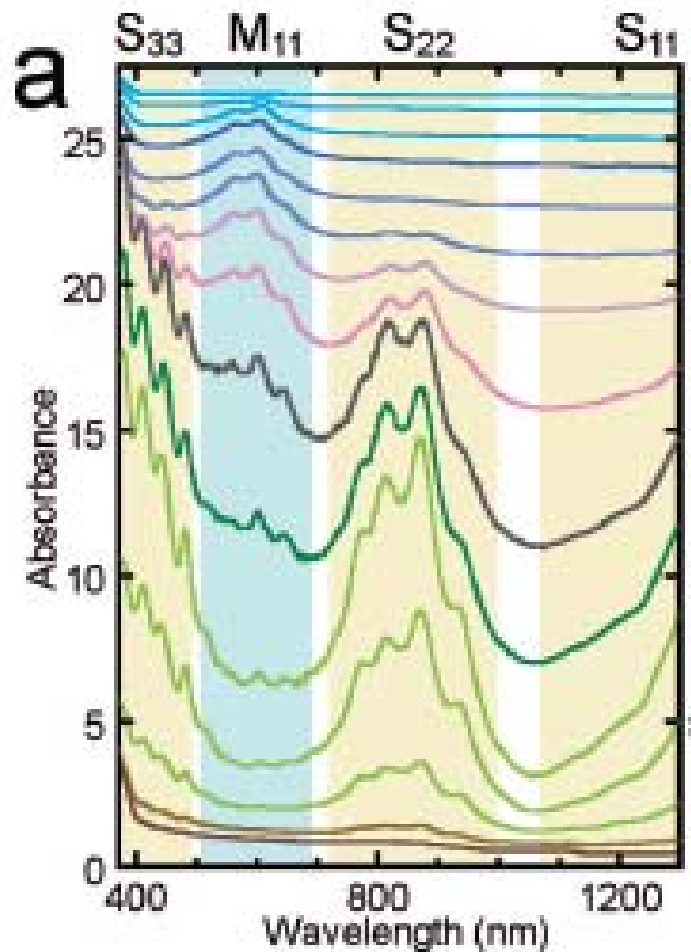


Figure 2:

Note: Molar absorptivity has units of $M^{-1}cm^{-1}$
Absorbance has no units.

How to Present the Scale for Multiple Spectra

Wrong Way



Right Way

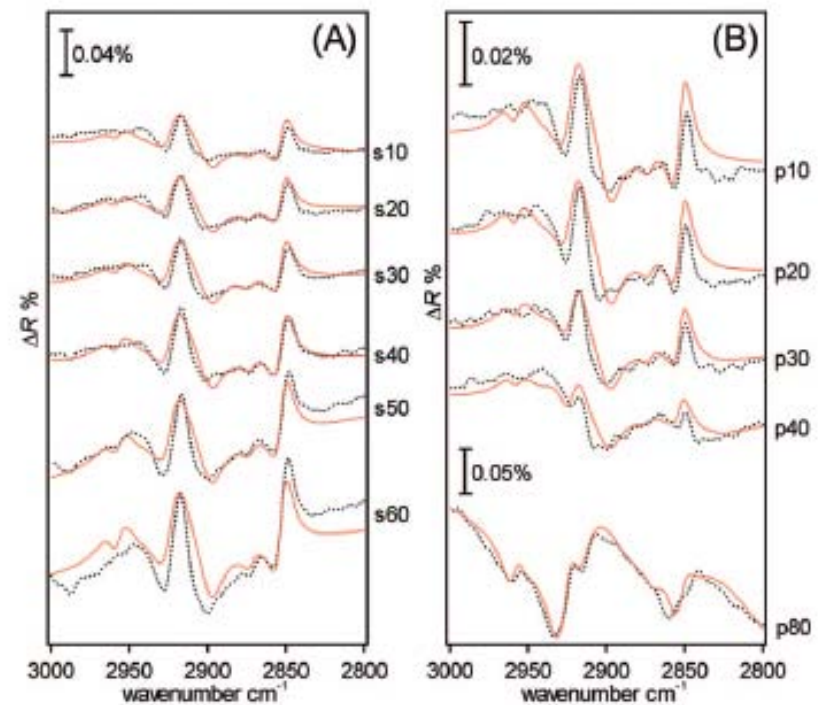
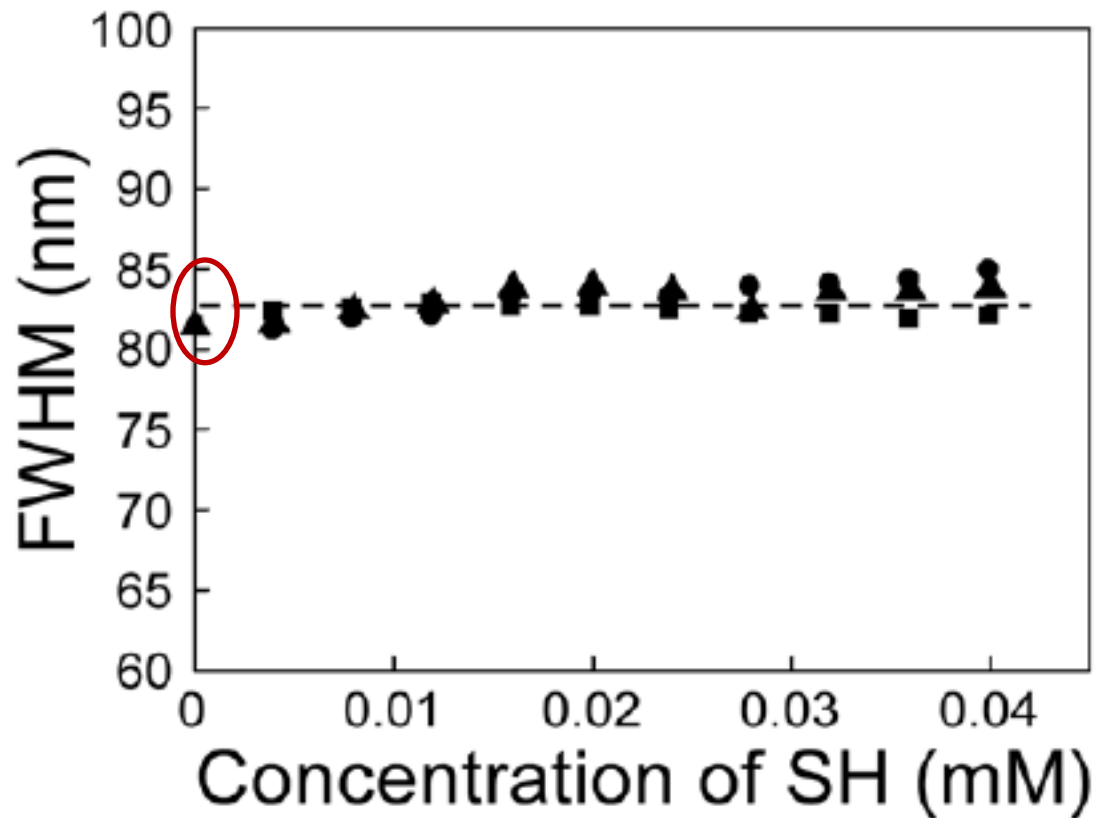


Figure 8. Subtracted spectra (dotted line) measured by s-polarization (A) and p-polarization (B) and their simulations (solid line). The IER spectra of 28.1 °C were subtracted from those of 24.7 °C measured at the same incident angle.

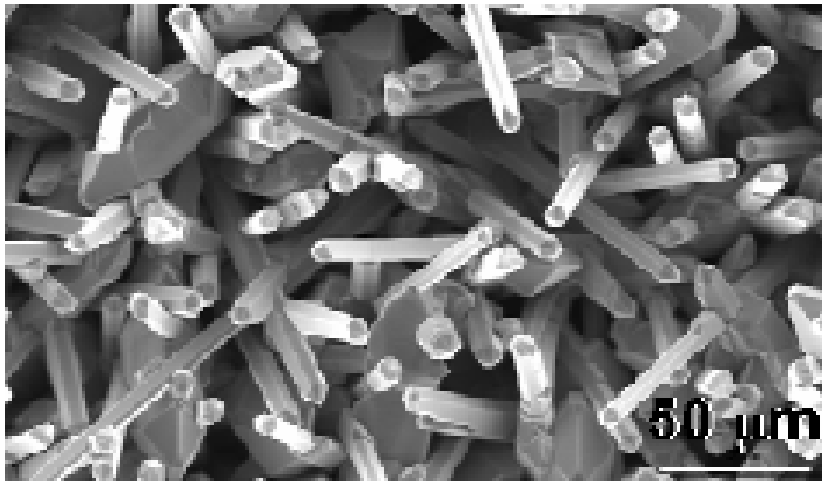
Select scale wisely

What can you conclude from this graph?

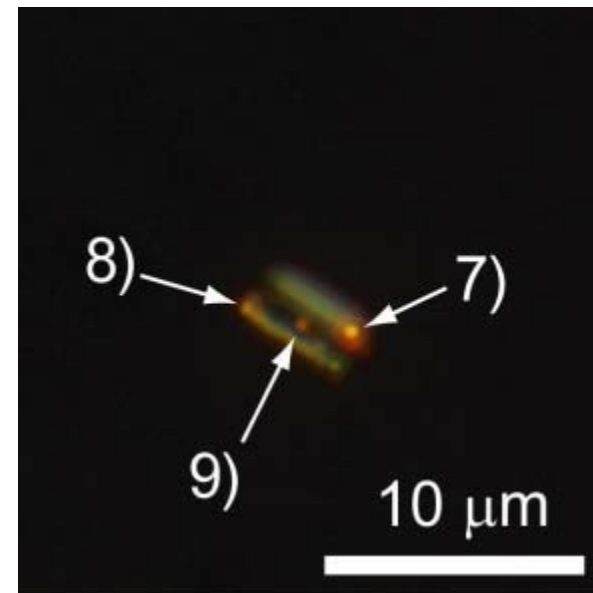


Scale bars in Micrographs

Illegible scale bars are a common problem



Scale bar clearly indicated



Scale bars in Micrographs

If font quality cannot be improved the size of the scale bar can be indicated in the caption. (Just don't forget to include it.)

Figure S4 FT-IR spectra of the prepared PANI-PPy nanofibers by a surfactant-assisted chemical oxidative copolymerization method with different molar ratios of aniline (An) and pyrrole (Py) monomers [An:Py], using cetyltrimethyl ammonium chloride (CTAC) as the surfactant.

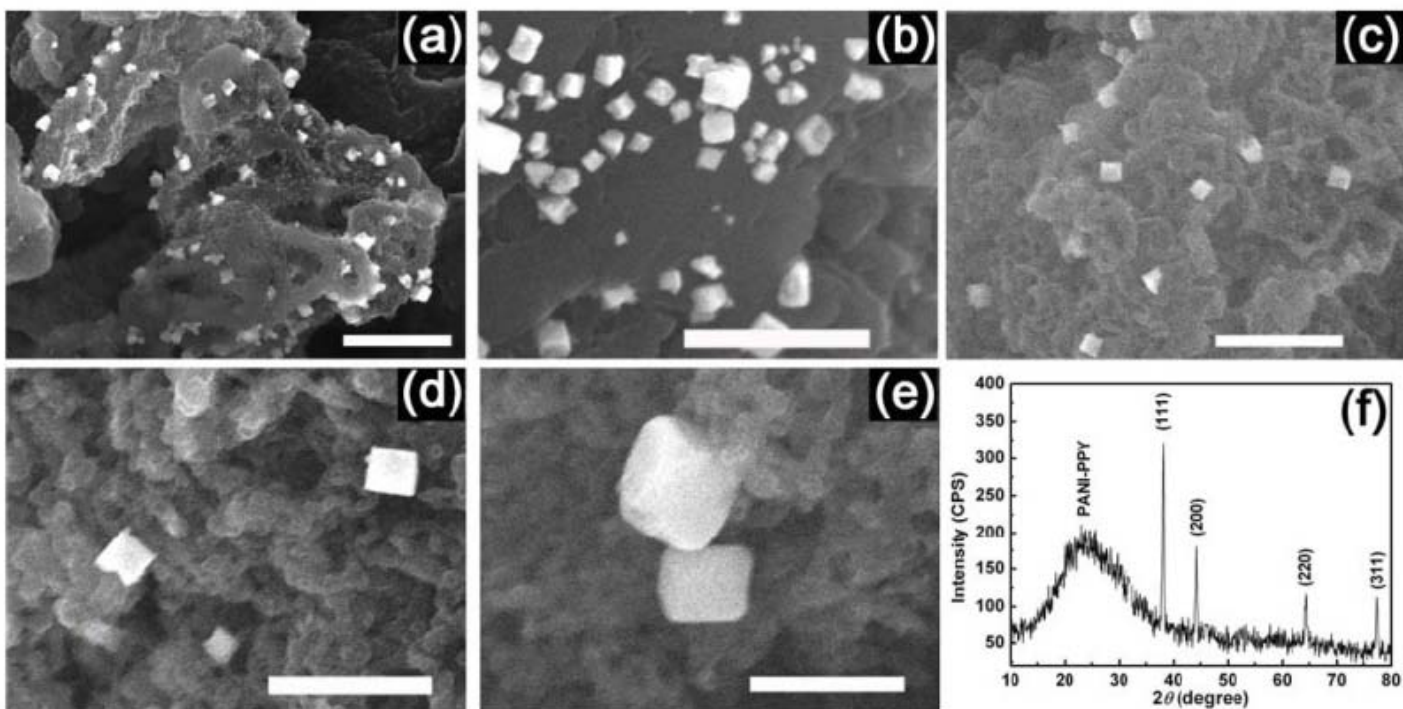


Figure S5 Magnification of Figure 2.

5. Check for Accuracy

(Proof your work! Typos can change the meaning.)

Author actually studied dGMP, a different chemical than GMP

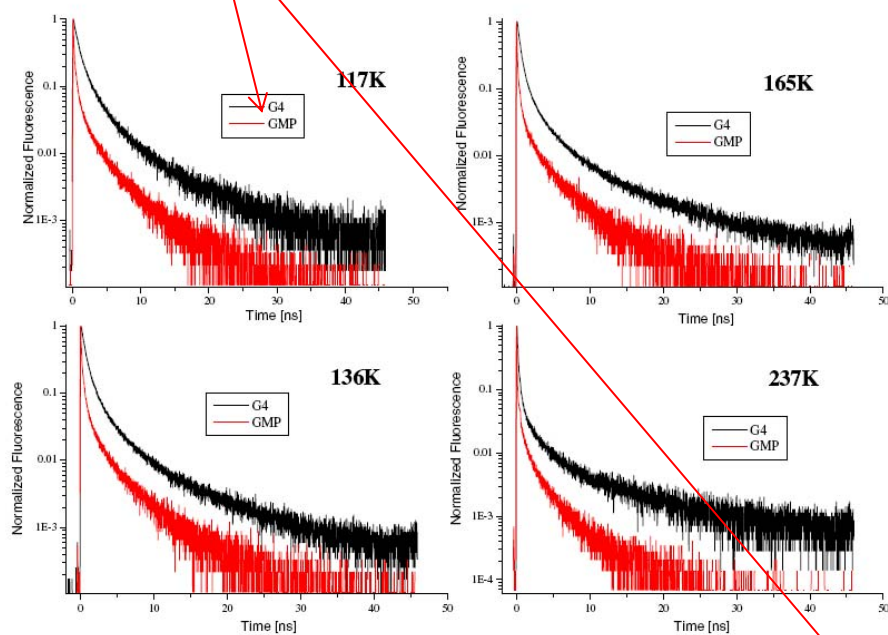


Fig 4a

Figure 4a. A semilog plot of the time resolved emission of G4 wires and dGMP in frozen aqueous solution at several temperatures.

Accurate Labeling

Which is the $\text{Na}_{0.7}\text{CoO}_2$ series?

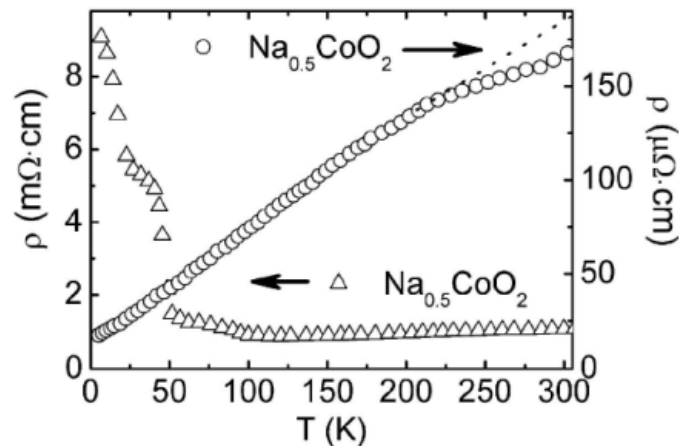
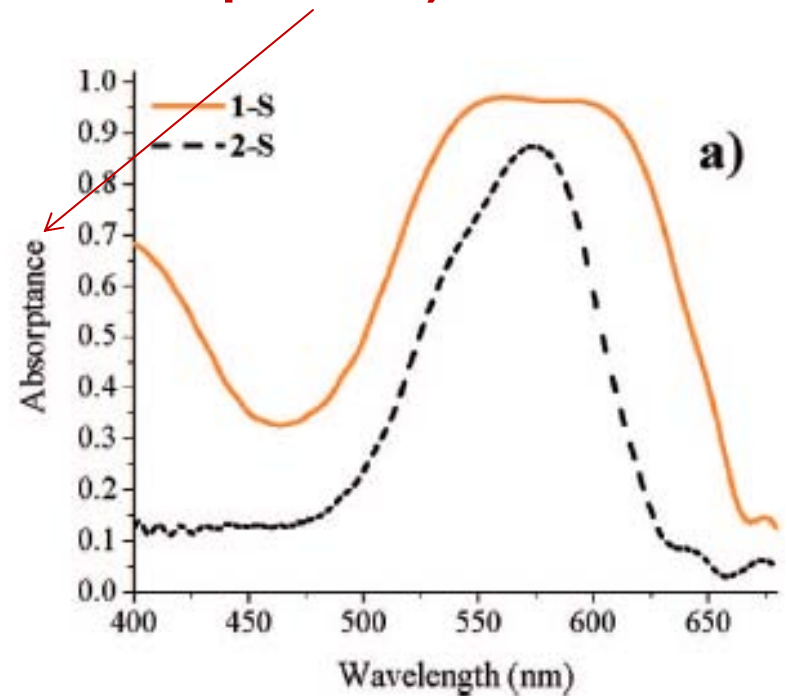


Figure 3

Resistivities of $\text{Na}_{0.5}\text{CoO}_2$ and $\text{Na}_{0.7}\text{CoO}_2$ thin films. The resistivity of $\text{Na}_{0.7}\text{CoO}_2$ thin film shows a “Curie-Wiess” metallic property similar to the resistivity of $\text{Na}_{0.7}\text{CoO}_2$ single crystal. The $\text{Na}_{0.5}\text{CoO}_2$ exhibits the transport behavior of a charge-ordered insulator.
98x82mm (600 x 600 DPI)

Do not “invent” new scientific terms (What is absorbance?)



Graphics Disguised as Figures

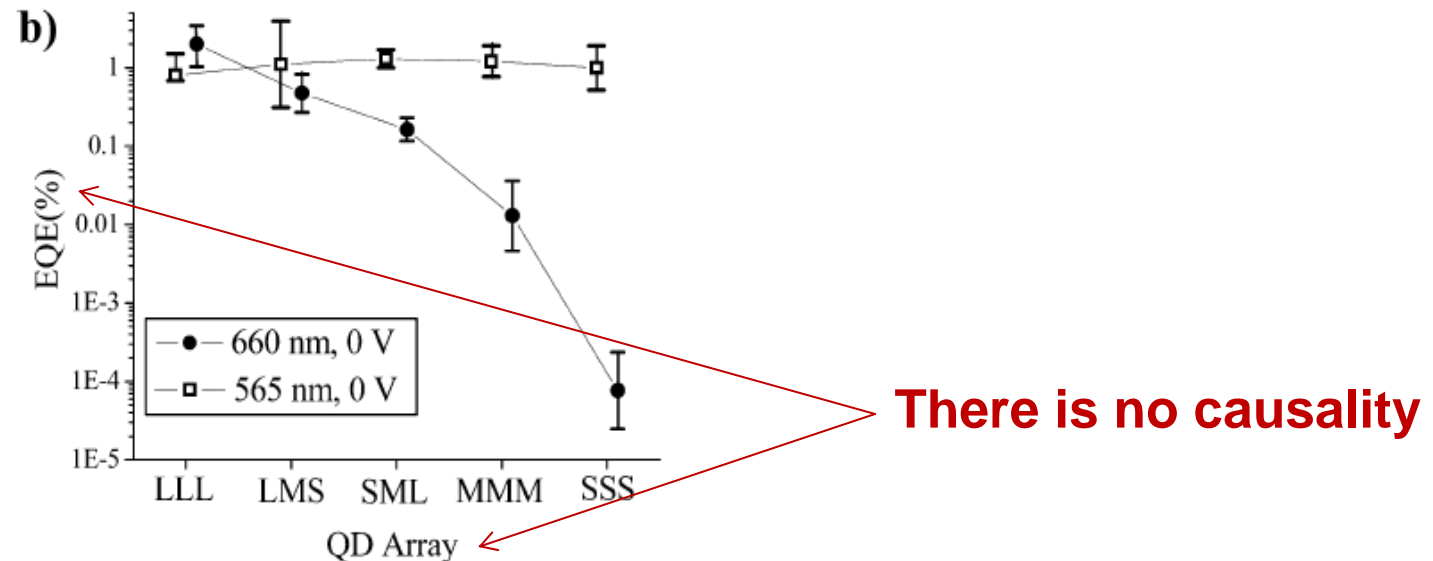
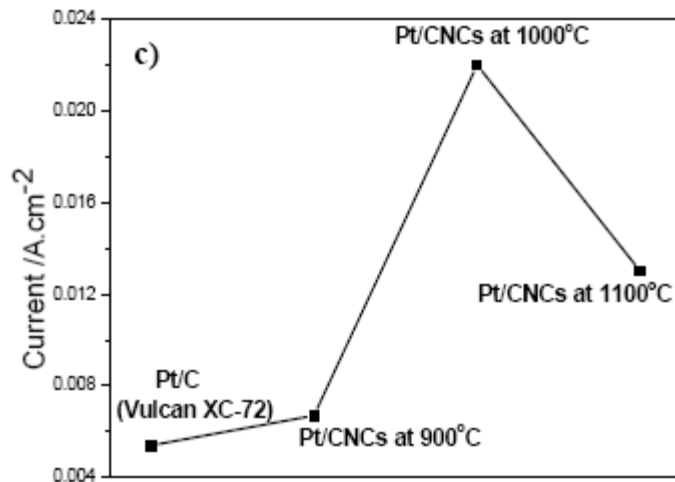


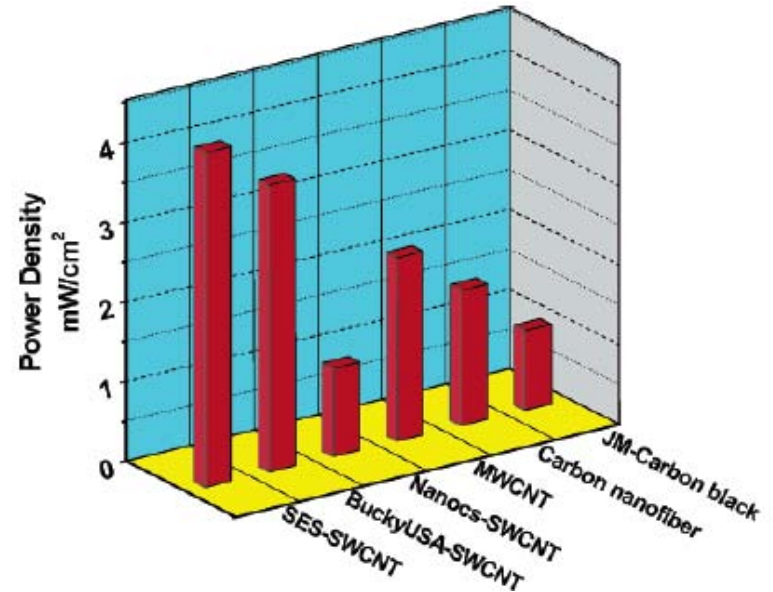
Figure 4. (a) Current–voltage (I – V) plots for the junction ITO/P/SSS/EGaIn in the dark (■) and with excitation (using LEDs) at 565 nm (▲) and 660 nm (○). The traces for the data taken in the dark and under illumination at 660 nm were hysteretic; the arrows show the direction in which we scanned V . (b) Plots of the external quantum efficiency (EQE, values are also listed in Table 1), defined as electrons that enter the external circuit per incident photon, at $V = 0$ V for ITO/P/X/EGaIn, X = LLL, LMS, MMM, SML, and SSS, with excitation (using LEDs) at 565 and 660 nm. The points for each array are offset along the x -axis for clarity. The lines connecting data obtained at a common wavelength are to guide the eye. The text contains the equation used to calculate EQE for our system, and the Supporting Information describes the calculation of the error bars.

“Graphs” that aren’t graphs

Is there a relationship between X and Y?



The right way to present non-causal data



A bar diagram can be used when comparing the performance of different samples

Summary (adapted from Tufte, pg 183)

Good graphic

- Terms are spelled out
- Text runs left to right
- Data are clarified with small notes
- Legends vs. labels –decide which one is appropriate
- Graphic attracts viewer
- Color choices (blue - good)
- Font type is clear, precise, modest
- Upper & lower case, with serifs
- Graphics should tend toward the horizontal, greater in length than height.

Bad graphic

- Excessive abbreviations to decode
- Text in vertical or multiple directions
- Graphic requires repeated references to scattered text
- Repeated back and forth between legend and graphic required
- Graphic is repellent, filled with chartjunk
- Dark letters on dark contrast (Red & green)
- Type is dense, heavy, overbearing
- All upper case, sans serif