Optical Modelling of Carbon Nano-Onions:
From Classical Extinction to Quantum Confinement

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Outlines

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- Project background
- Single CNO
- Aggregates
- Laser heating
- AI agent

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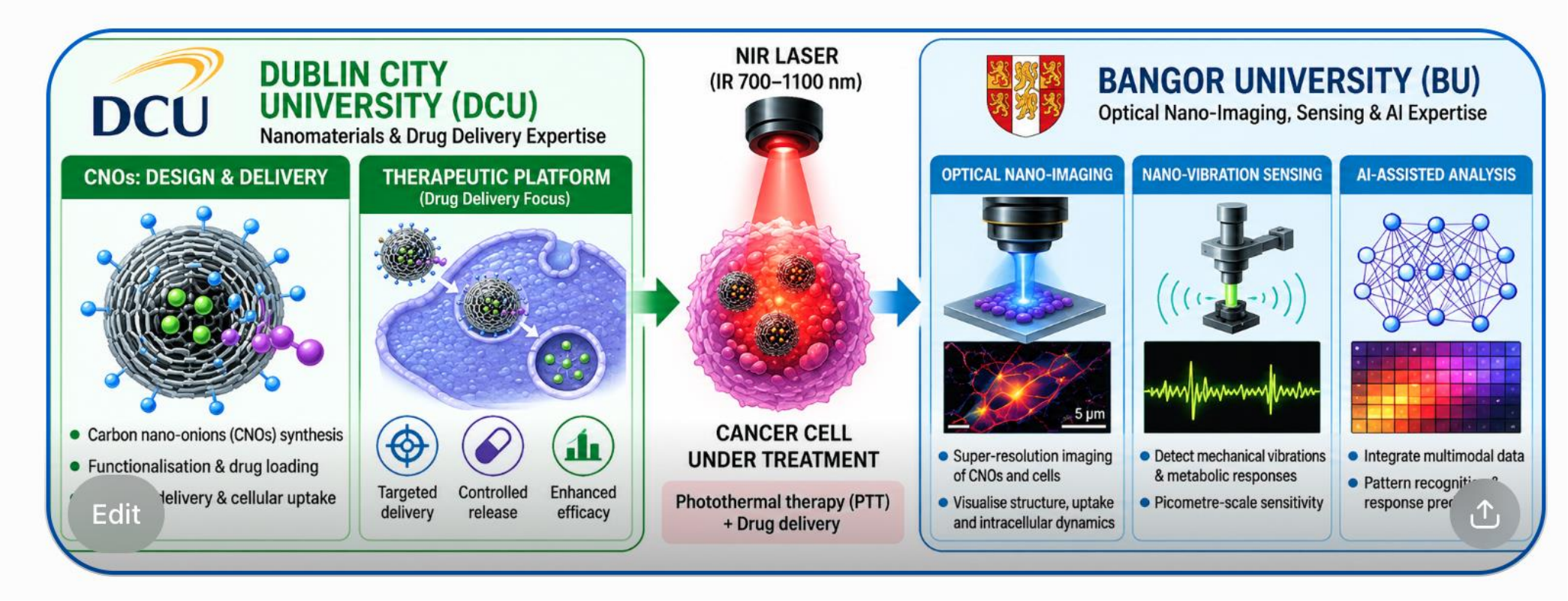
Wales Innovation Network
Rhwydwaith Arloesi Cymru

Background:

1) Feasibility study on CNO for Photo Thermal Therapy (PTT)
   establish foundation for dual therapy (drug delivery + PTT) approach

2) Theoretical modelling of CNO optical properties



2. Photo Thermal Therapy (PTT)

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- **Principle:** Converts laser light into heat via light-absorbing agents to selectively destroy cancer cells (42–47 °C for hyperthermia; >48 °C for ablation).

- **Carbon Nanomaterials as Transducers:** Carbon nano-onions (CNOs), CNTs, graphene/oxide, fullerenes, and carbon dots offer **broadband optical absorption**, high **chemical stability**, and **biocompatibility**.

- **Advantage over Metals:** Unlike plasmonic metals (e.g. Au) with narrow absorption peaks, carbon materials absorb across a wide spectrum (“black”), enabling multi-wavelength operation.

- **Typical Lasers:** 785, 808, and 1064 nm (CW or pulsed) maximize intratumoral heating.

ACS APPLIED NANO MATERIALS

www.acsanm.org Article

Controlled Phase Transition of the Onion-like Carbon Nanostructure for Photothermal Cancer Therapy

Yuchen Feng,[#] Siyi Lu,[#] Qi Zhao,[*] Tianyang Sun, Yuxi Shi, Guanyue Gao, Hao Wang,[*] and Jinfang Zhi[*]

Cite This: *ACS Appl. Nano Mater.* 2024, 7, 7008−7017 Read Online

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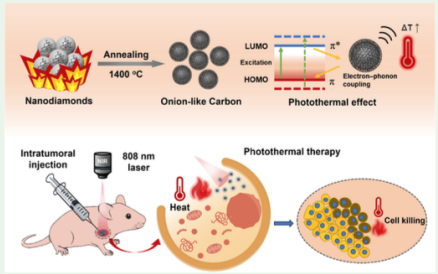
ABSTRACT: Carbon-based nanomaterials are viewed as preferred candidates as photothermal agents in tumor photothermal therapy due to their tailored structure and excellent biocompatibility. Herein, onion-like carbon (OLC) with controlled sp^2/sp^3-hybridized carbon ratios was explored as an effective photothermal reagent. The OLC was synthesized through thermal annealing of nanodiamonds, with an increase of the sp^2 carbon content as the annealing temperature increased. The obtained OLC demonstrated high photothermal efficiency under 808 nm laser irradiation with a maximum value of 74.36% at an annealing temperature of 1400 °C. We suggest that a well-regulated amount of sp^2 carbon in the OLC provided an abundance of conjugated π bonds, leading to enhanced light absorption and electron−phonon coupling. In addition, the OLC was conjugated with polyethylene glycol (PEG) and fluorescent molecules (FITC) to visualize the cellular uptake in HCT 116. In vivo tests demonstrated that the OLC-PEG-FITC exhibited good biocompatibility and achieved photothermal killing of cancer cells upon near-infrared laser irradiation. After treatment with the OLC-based photothermal agent, tumor tissues in tumor-bearing mice were effectively ablated. Taken together, these findings confirm the potential of the developed OLC as a photothermal agent for tumor therapy.



KEYWORDS: *onion-like carbon, sp^2 carbon, nanostructure fabrication, photothermal effect, tumor therapy*

OLC, 808nm laser, 74.36% photothermal efficiency

CHEMICAL REVIEWS

pubs.acs.org/CR Review

Photothermal Nanomaterials: A Powerful Light-to-Heat Converter

Ximin Cui,[†] Qifeng Ruan,[†] Xiaolu Zhuo,[†] Xinyue Xia, Jingtian Hu, Runfang Fu, Yang Li, Jianfang Wang,[*] and Hongxing Xu[*]

Cite This: *Chem. Rev.* 2023, 123, 6891−6952 Read Online

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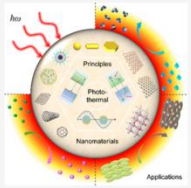
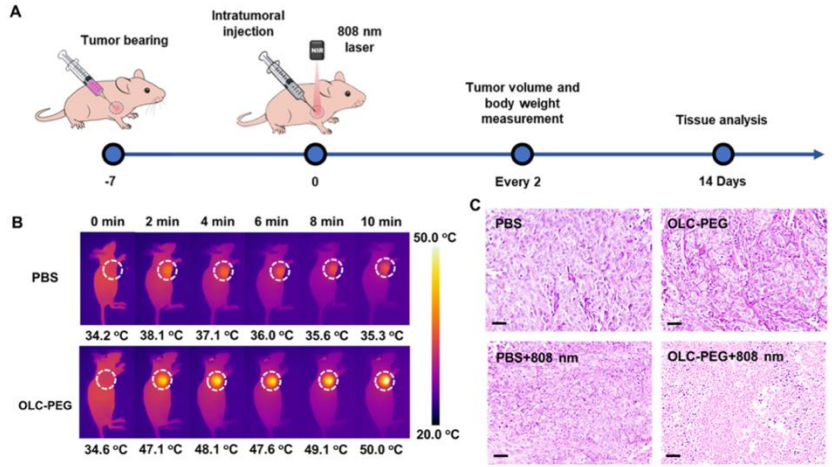
ABSTRACT: All forms of energy follow the law of conservation of energy, by which they can be neither created nor destroyed. Light-to-heat conversion as a traditional yet constantly evolving means of converting light into thermal energy has been of enduring appeal to researchers and the public. With the continuous development of advanced nanotechnologies, a variety of photothermal nanomaterials have been endowed with excellent light harvesting and photothermal conversion capabilities for exploring fascinating and prospective applications. Herein we review the latest progresses on photothermal nanomaterials, with a focus on their underlying mechanisms as powerful light-to-heat converters. We present an extensive catalogue of nanostructured photothermal materials, including metallic/semiconductor structures, carbon materials, organic polymers, and two-dimensional materials. The proper material selection and rational structural design for improving the photothermal performance are then discussed. We also provide a representative overview of the latest techniques for probing photothermally generated heat at the nanoscale. We finally review the recent significant developments of photothermal applications and give a brief outlook on the current challenges and future directions of photothermal nanomaterials.





Literature

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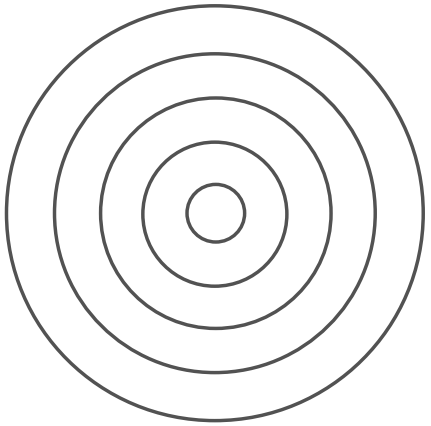
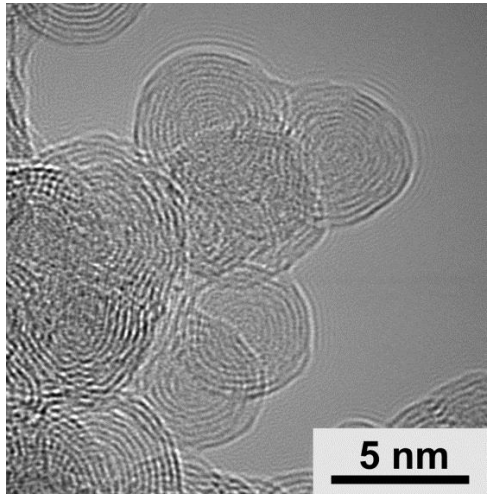
Carbon Nanomaterial	Representative Morphology	Laser Conditions / Notes	Typical ΔT or Observed Heating	Representative PCE Range / Value	Representative Source(s)
Graphene / rGO	2D sp^2 sheets	808 nm, ~1 W cm^{-2} (in many studies)	30–40 °C rise (in many reports)	~ 45–60 % (varies)	Summarized in Cui et al., *Chem. Rev.* 2023 (citing original graphene PTT studies) ACS Publications
Carbon Nanotubes (CNTs)	1D tubular sp^2	808 nm, ~1 W cm^{-2} (in many reports)	25–35 °C	~ 40–50 %	Summarized in Cui et al., *Chem. Rev.* 2023 ACS Publications
Carbon Dots (CDs / CQDs)	Nanoparticles, sp^2/sp^3 mix	808 nm (or NIR)	15–25 °C (in many studies)	~ 25–40 %	Summarized in Cui et al., *Chem. Rev.* 2023 ACS Publications
Nanodiamonds (NDs)	sp^3 cubic	Various lasers in literature	<10 °C (weak heating)	< ~ 10 %	Summarized in Cui et al., *Chem. Rev.* 2023 ACS Publications
Onion-Like Carbon (OLC / CNO)	Concentric graphitic shells	808 nm, 1.75 W cm^{-2} (in Feng et al. work)	~35 °C rise (for best sample)	**74.36 %**	Feng et al., *ACS Applied Nano Materials* 2024 ACS Publications

CNO is the best for PTT

Carbon nano-onions (CNO) : the object we model



concentric graphitic shells



Single CNO: 5-6 nm, sp^2-rich shells

- CNOs consist of concentric graphitic shells formed by annealing nanodiamonds.
- Increasing temperature (900–1400 °C) drives $sp^3 \rightarrow sp^2$ transition.
- Enhanced π-electron delocalization improves absorption across UV–Visible–NIR.

Higher sp^2 content → stronger light absorption and heat conversion.

DCU: Pristine (pCNO) vs Oxidized (oCNO)

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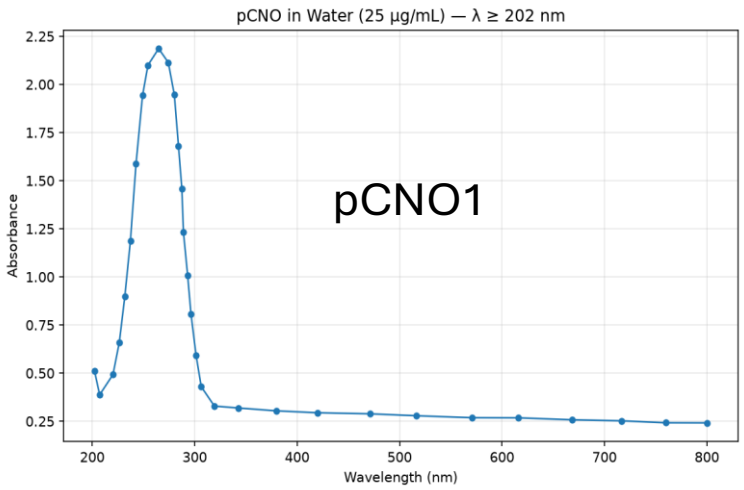
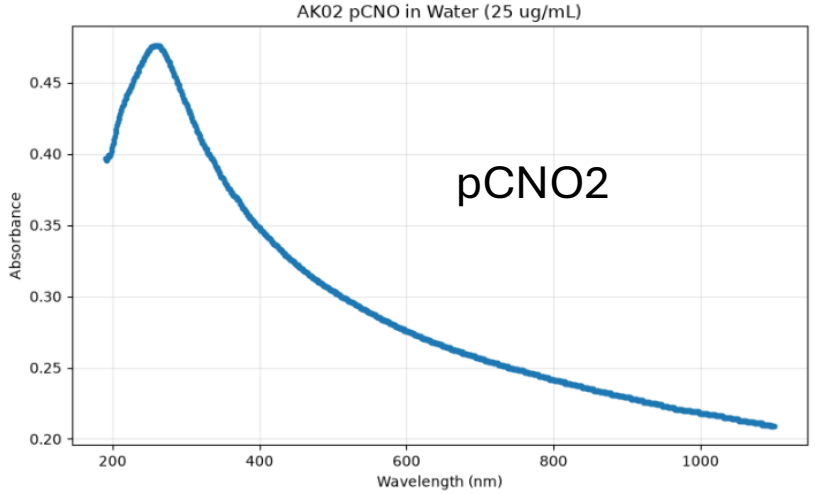
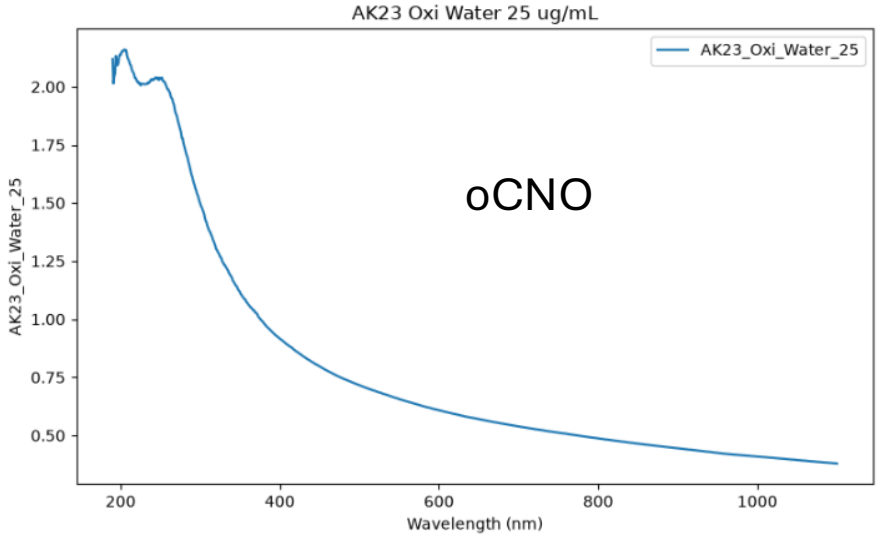
- **pCNO:** single peak **256 nm**
- **oCNO:** double peaks at **244 nm** and **205 nm**

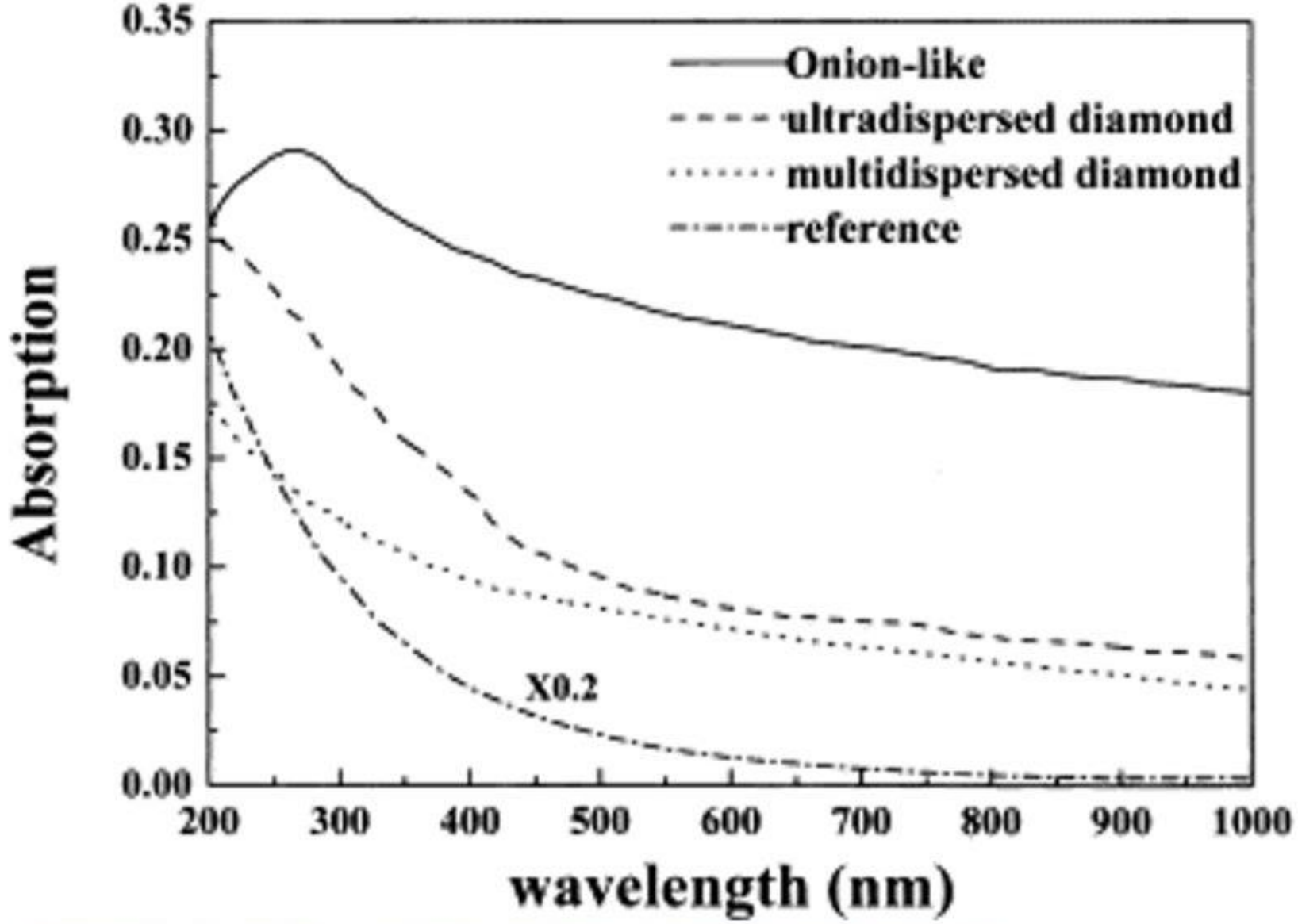






Goal: Develop a model to explain the spectrum

Other group:



https://www.sciencedirect.com/science/article/pii/S0009261402005572

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UV–Visible Absorption in CNOs

1 UV region (200–350 nm)

- Strong $\pi \rightarrow \pi^*$ transition from sp^2 carbon
- $\sigma \rightarrow \sigma^*$ contribution at shorter UV wavelengths
- Main UV peak linked to graphitic shells

2 Visible–NIR region (400–900 nm)

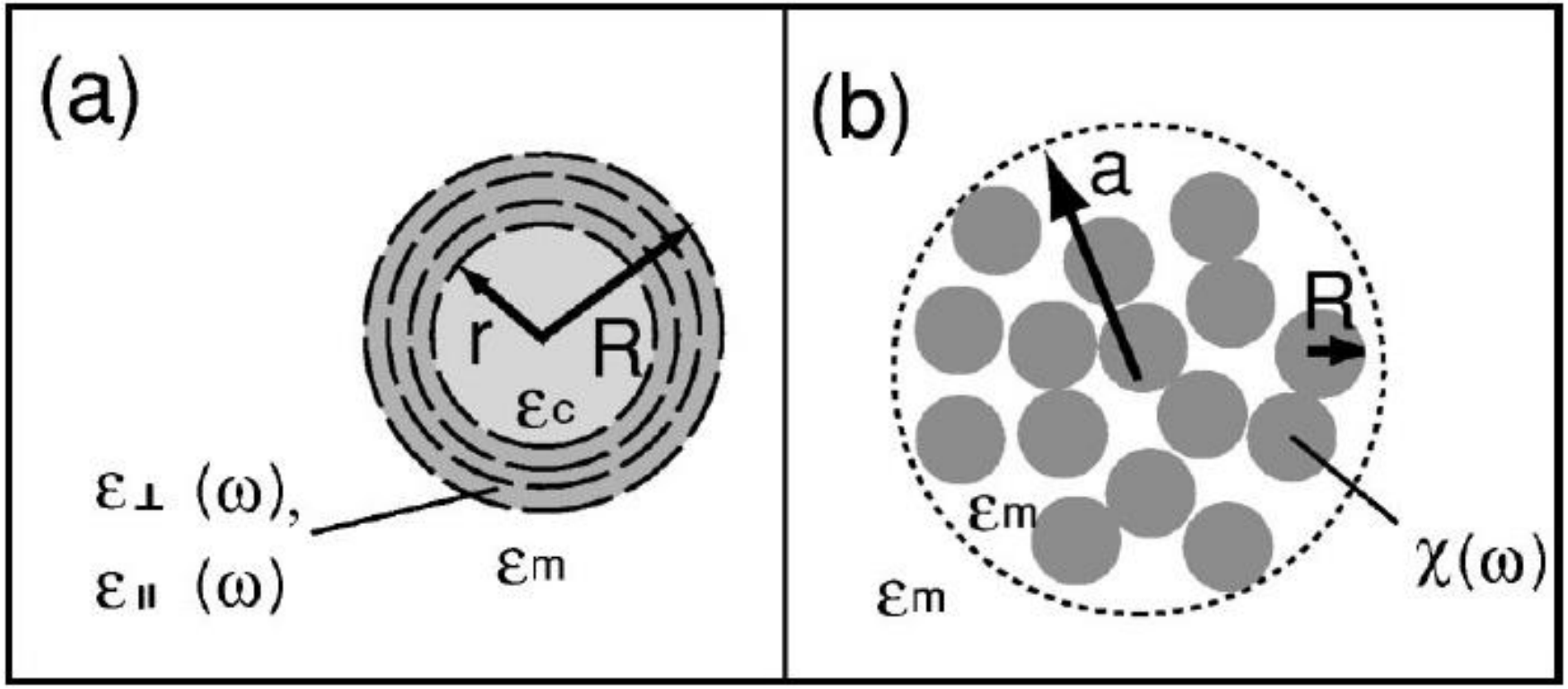
- Broad weaker absorpition tail
- Caused by defects, curvature and shell coupling
- Enables response beyond the UV peak

3 Why 808 nm matters

- No sharp 808 nm peak is required
- The long-wavelength tail still absorbs NIR light
- Absorbed energy is converted into heat for photothermal therapy

Key message: UV dominates the spectrum, while the weaker NIR tail enables photothermal heating.

Modelling Geometry



Single

Aggregate
(hydrodynamic size)

Classical baseline: carbon-onion extinction

Tomita-style carbon onion calculations motivate the single-particle starting point

PHYSICAL REVIEW B **66**, 245424 (2002)

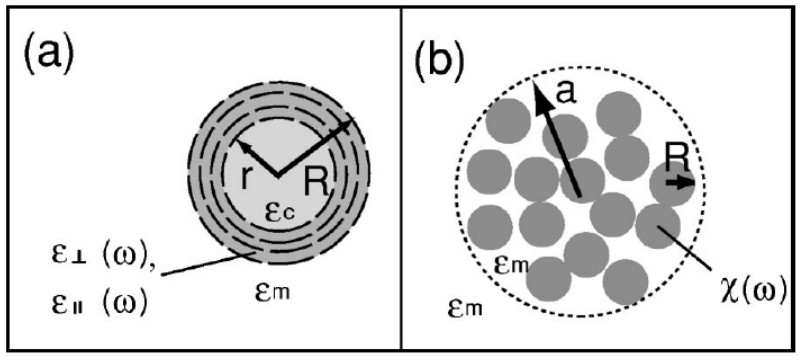


FIG. 3. Schematic illustrations of (a) a defective spherical onion with core material and (b) an aggregate of the onions.

PHYSICAL REVIEW B **66**, 245424 (2002)

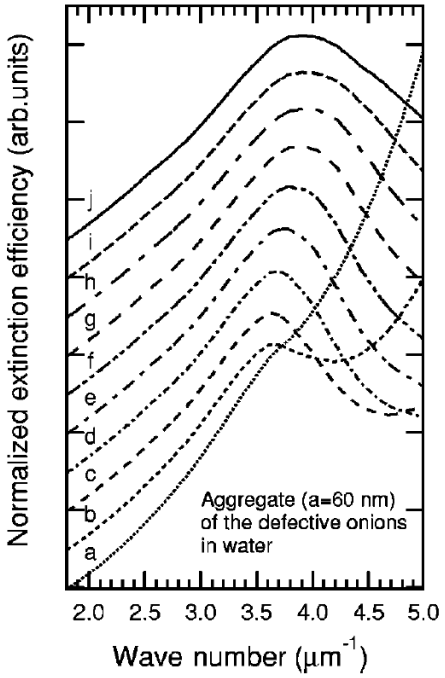


FIG. 6. Calculated extinction spectra for an aggregate (a = 60 nm) of defective spherical onions in water. The parameters for the defective onions used here are the same ones as in Fig. 4.

- *Tomita, Satoshi, Minoru Fujii, and Shinji Hayashi. "Optical extinction properties of carbon onions prepared from diamond nanoparticles." Physical Review B 66.24 (2002): 245424.*
- *Tomita, S., et al. "Ultraviolet-visible absorption spectroscopy of carbon onions." Physics of the Solid State 44.3 (2002): 450-453.*

pyMieCNO code map

What is actually calculated in the implementation

Spectrum_single.py

single-CNO core–shell polarizability
isotropic / anisotropic / quantum

materials_config.py

R = 3 nm; cases a–f
quantum parameters for pCNO/oCNO

Spectrum_porous.py

Maxwell–Garnett EMT
porous aggregate effective n,k

utils/fv_fit.py

fit f_v against UV–Vis with DLS curve or lognormal size

laser_heating.py

A808 + η → T(t)
0-D bulk heat balance

CNO shell physics → inclusion optical constants → porous aggregate effective n,k → DLS-weighted Mie extinction → fitted UV–Vis spectrum

Important modelling interpretation

The solvent is treated as the matrix inside the porous cluster. The fitted f_v is the CNO solid volume fraction in the hydrodynamic aggregate.

Quantum model — core spectral transform

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Three adjustable terms: shell permittivity, spectral narrowing, and peak shift

1 Shell permittivity

Replaces the fixed 2/3 : 1/3 Voigt average with a fitted in-plane weighting factor.

$$\varepsilon_{\text{shell}} = w\,\varepsilon_{\parallel} + (1-w)\,\varepsilon_{\perp}$$

w = fitted in-plane weight

2 Spectral narrowing

Map wavelength onto a narrowed coordinate, interpolate k(λ), then renormalize absorption.

$$\lambda' = \lambda_{\text{peak}} + \frac{\lambda - \lambda_{\text{peak}}}{\gamma}$$

$\gamma < 1$ narrows $\quad$ $\gamma > 1$ broadens

3 Peak shift

Evaluate optical constants at a shifted wavelength to move the whole spectrum.

$$n, k: \quad \lambda \to \frac{\lambda}{\delta}$$

$\delta > 1$ red-shift $\quad$ $\delta < 1$ blue-shift

Modelling workflow

$$\varepsilon_{\text{shell}} \longrightarrow k(\lambda') \longrightarrow C_{\text{abs}}(\lambda;\gamma,\delta)$$

Renormalize to conserve total absorption after narrowing / broadening.

Purpose: keep the physics interpretable while allowing the model to fit shifted and broadened CNO spectra.

Quantum model — absorption corrections

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Separate physically motivated corrections from baseline and oxidation effects

4 Far-UV Gaussian band

Added on top of the shifted/narrowed spectrum to capture extra far-UV absorption.

$$\Delta C_{\mathrm{abs}}^{\mathrm{UV}} = A_{\mathrm{UV}}\, C_{\mathrm{abs},\,peak}\, \exp\left[-\frac{1}{2}\left(\frac{\lambda-\lambda_{\mathrm{UV}}}{\nu_{\mathrm{UV}}}\right)^2\right]$$

5 Background continuum

Two independent power-law components describe the slowly varying tail.

$$C_{\mathrm{abs}}^{\mathrm{bg}} = A_1\left(\frac{\lambda}{800\,\mathrm{nm}}\right)^{-p_1} + A_2\left(\frac{\lambda}{800\,\mathrm{nm}}\right)^{p_2}$$

6 Oxidized CNO only

Extra C=O / COOH surface-state contribution added directly to aggregate polarizability.

$$\Delta\alpha_{\mathrm{CO}} = A_{\mathrm{CO}}\, V\, \exp\left[-\frac{1}{2}\left(\frac{\lambda-205\,\mathrm{nm}}{10\,\mathrm{nm}}\right)^2\right]$$

Clean separation of effects

- **Core spectrum:** εshell, γ, δ
- **Added absorption:** UV band + continuum
- **Oxidation signature:** C=O / COOH term only for oCNO

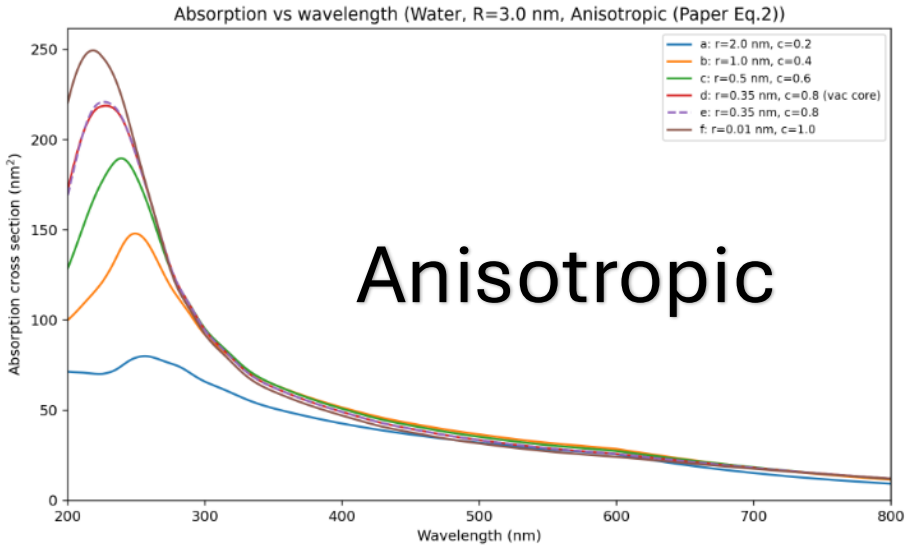
This makes each fitting parameter easier to explain during the talk.

Quantum Model — Fitted Parameters (pCNO vs oCNO)

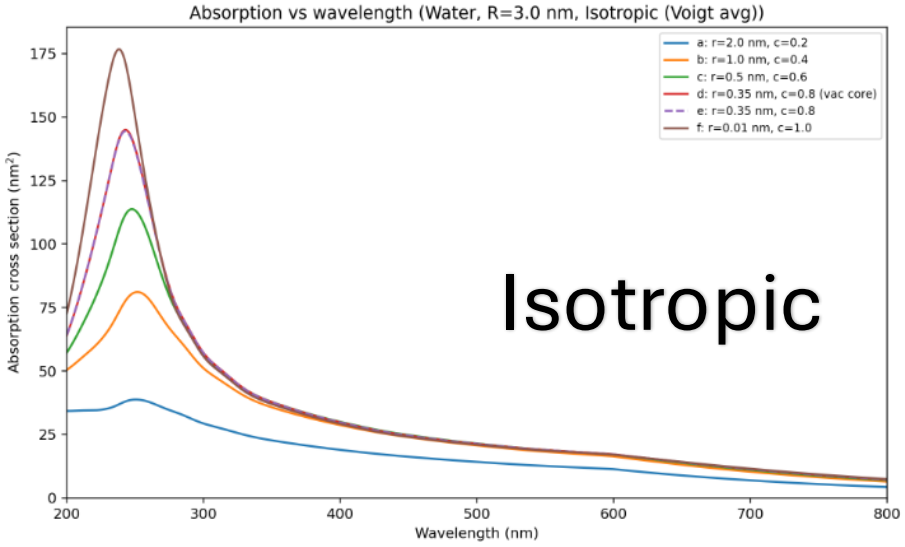
Parameter	pCNO	oCNO	Physical meaning
w (in-plane weight)	0.968	0.968	Same graphiticity -- pi-pi* transition present in both
gamma (narrowing)	1.40	1.40	Same spectral narrowing -- sharp UV peak in both
delta (peak shift)	1.02	1.00	pCNO ~2% red-shifted; oCNO unshifted (aggregate MG shift instead)
bg_amp / bg_power	0.10 / 1.5	0.10 / 1.5	UV-side background uplift (same form both cases)
bg2_amp / bg2_power	0.25 / 0.0	0.00 / 0.0	Long-wavelength flat tail -- only needed for pCNO
co2_amp (extra term)	n/a	1.70	C=O/COOH surface absorption, centered 205 nm, width 10 nm

Base parameters from materials_config.py (w, gamma, delta act on the single-particle shell, bg2_amp/co2_amp are applied at the aggregate level.

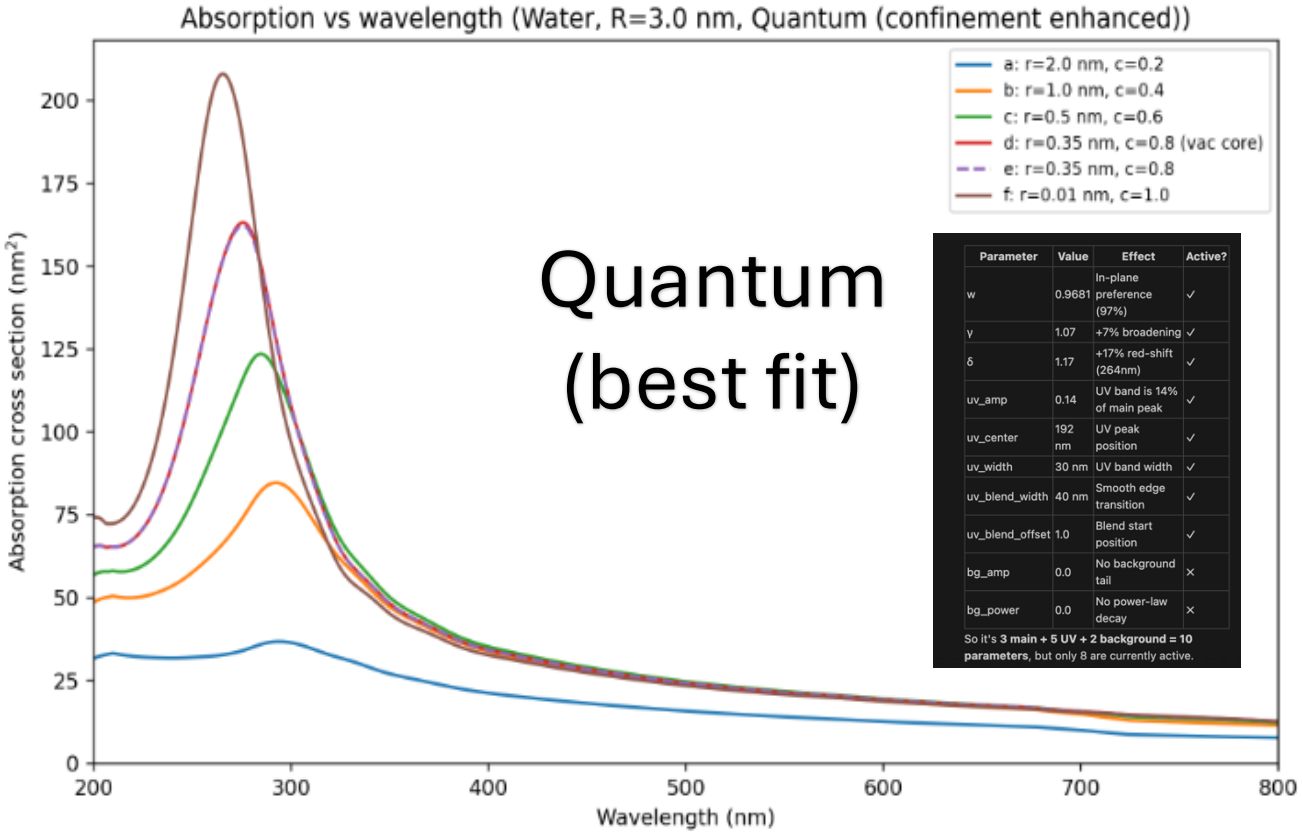
Single CNO model



python Spectrum_single.py --medium Water --model-type anisotropic



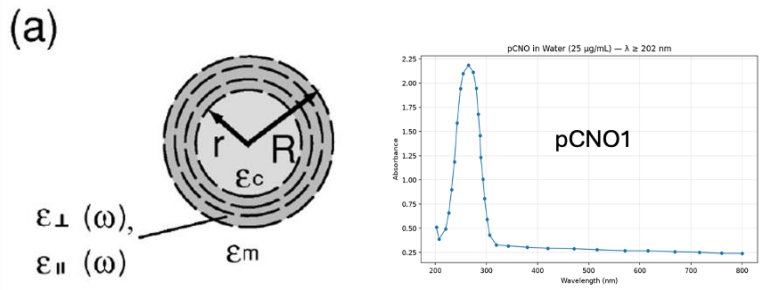
python Spectrum_single.py --medium Water --model-type isotropic



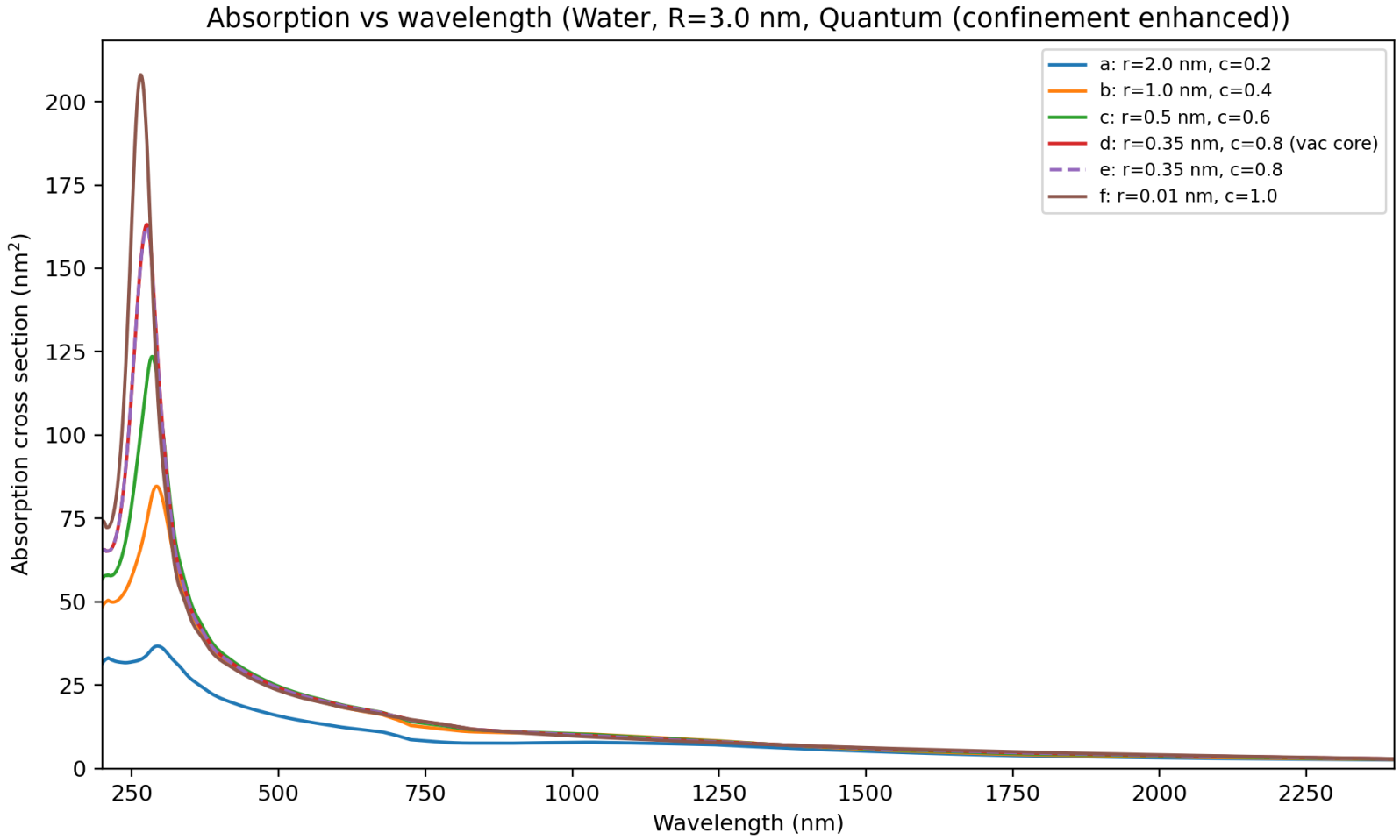
Parameter	Value	Effect	Active?
w	0.9681	In-plane preference (97%)	✓
γ	1.07	+7% broadening	✓
δ	1.17	+17% red-shift (264nm)	✓
uv_amp	0.14	UV band is 14% of main peak	✓
uv_center	192 nm	UV peak position	✓
uv_width	30 nm	UV band width	✓
uv_blend_width	40 nm	Smooth edge transition	✓
uv_blend_offset	1.0	Blend start position	✓
bg_amp	0.0	No background tail	×
bg_power	0.0	No power-law decay	×

So it's **3 main + 5 UV + 2 background = 10 parameters**, but only 8 are currently active.

python Spectrum_single.py --medium Water --model-type Quantum

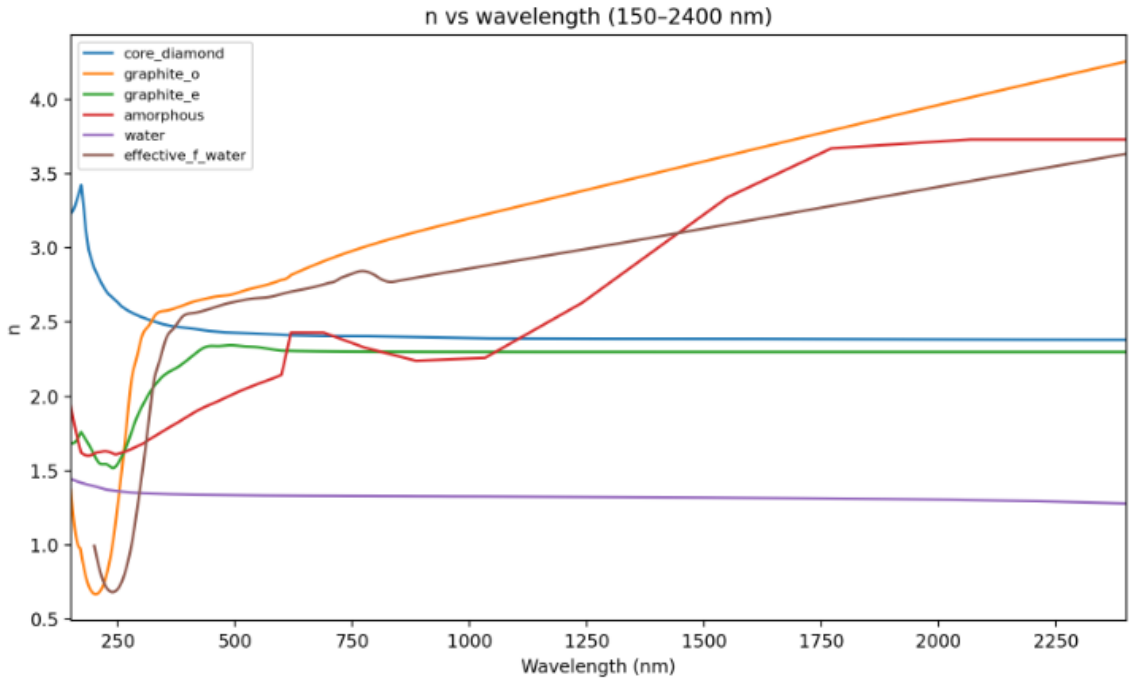


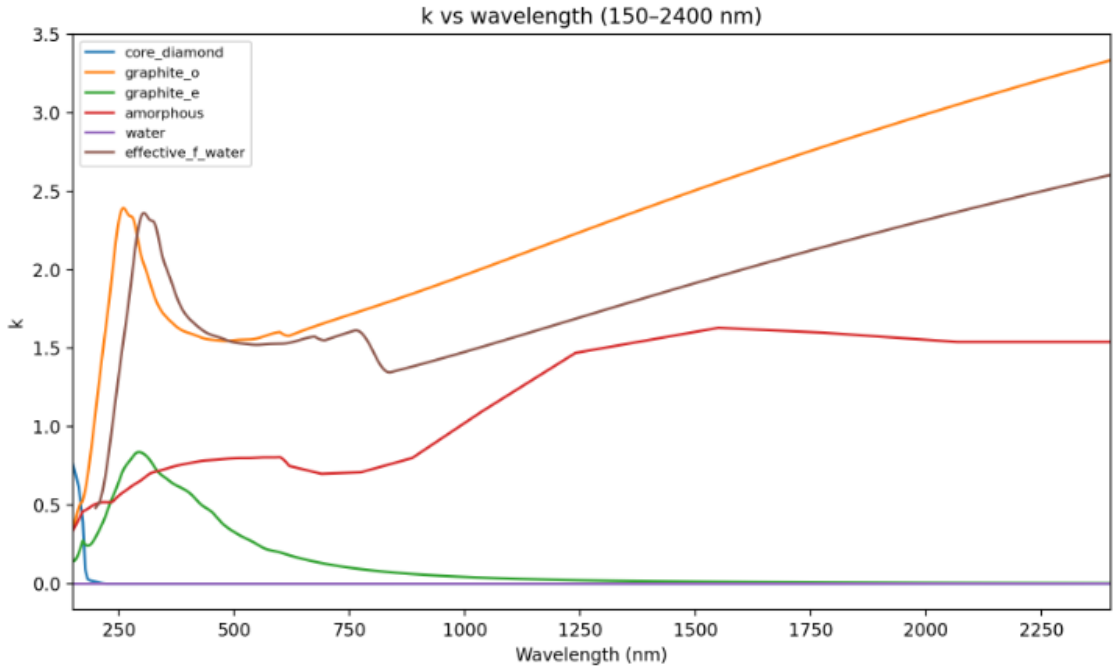
200-2400nm



Nothing special beyond 800nm to 2400nm, suggesting shorter wavelength is always preferred

Calculated Effective nk – ‘f’





Aggregate model: DLS gives size, EMT gives the optical interior

This is the most important bridge from single CNO to dispersion UV–Vis

Host solvent

mhost(λ) from Water / DMSO / NMP / Ethanol n,k

CNO inclusion

mincl(λ) from quantum single-CNO model or effective-nk CSV

Porous aggregate

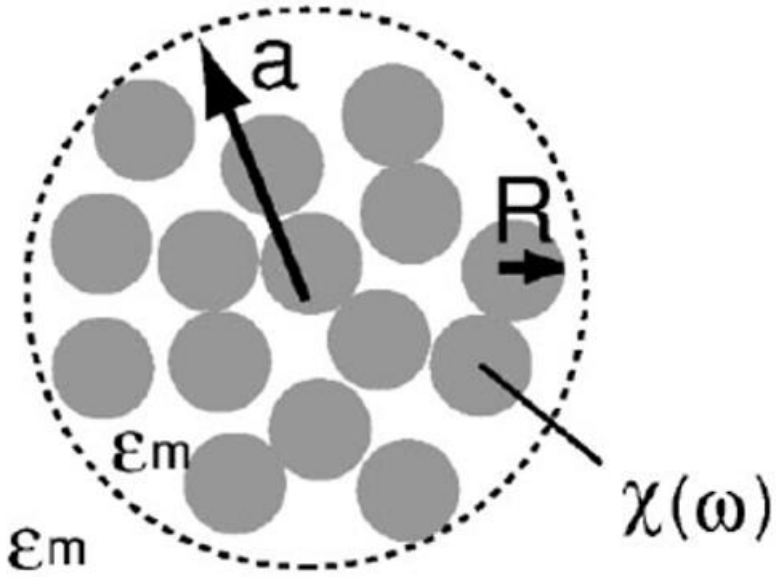
Maxwell–Garnett mixes solvent + CNO using f_v

Mie sphere

meff(λ) assigned to hydrodynamic aggregate

Interpretation of f_v

f_v is the CNO solid volume fraction in the hydrodynamic aggregate; porosity is 1 − f_v and is filled by solvent.



“DLS gives the outside size; Maxwell–Garnett gives what the porous inside looks like optically.”

Aggregate effective n,k: Maxwell–Garnett mixing in the code

Spectrum_porous.py → maxwell_garnett_effective_ri()

Host solvent $m_{host}(\lambda)$ — **CNO inclusion** $m_{incl}(\lambda)$ — **Volume fraction** f_v — **Effective medium** $\varepsilon_{eff}(\lambda)$ — **Output** n_{eff}, k_{eff}

Maxwell–Garnett equation

$$\beta = (\varepsilon_{incl} - \varepsilon_{host}) / (\varepsilon_{incl} + 2\varepsilon_{host})$$

$$\varepsilon_{eff} = \varepsilon_{host} \cdot (1 + 3 f_v \beta) / (1 - f_v \beta)$$

Physical meaning: CNO inclusions are embedded in a solvent-filled porous aggregate.

Convert ε to n,k

$$\varepsilon_{host} = m_{host}^2$$

$$\varepsilon_{incl} = m_{incl}^2$$

$$m_{eff}(\lambda) = \sqrt{\varepsilon_{eff}}$$

Then m_eff = n_eff + i k_eff; k is clipped to ≥ 0 after interpolation.

What f_v controls

Optical contrast + material density inside each hydrodynamic aggregate.

What is fitted

f_v changes the generated n,k; n,k itself is not fitted independently.

Speaker line

“DLS gives the outside size; MG gives the porous optical interior.”

From effective n,k to UV–Vis: DLS-weighted Mie ensemble

Implemented in Spectrum_porous.py calculate_spectrum()

1. Size distribution

Use DLS diameter bins + number fractions, or a lognormal distribution from Dg and σg.

2. Number concentration

C is CNO mass concentration, not aggregate mass.
$N \propto C / (f_v \rho_{CNO} E[D^3])$.

3. Mie loop

For each wavelength and size bin: Qext, Qsca, Qabs are computed using m_eff(λ).

Key physical point

Changing f_v changes both the aggregate effective n,k and the number of hydrodynamic aggregates for a fixed CNO mass concentration. This is why f_v is a strong fitting parameter.

DLS caveat

Large DLS tails may cause artificial resonances if treated as compact spheres; the code includes optional truncation to reduce this artefact.

DLS input: hydrodynamic aggregates, not primary CNOs

Measured size distributions constrain the ensemble calculation

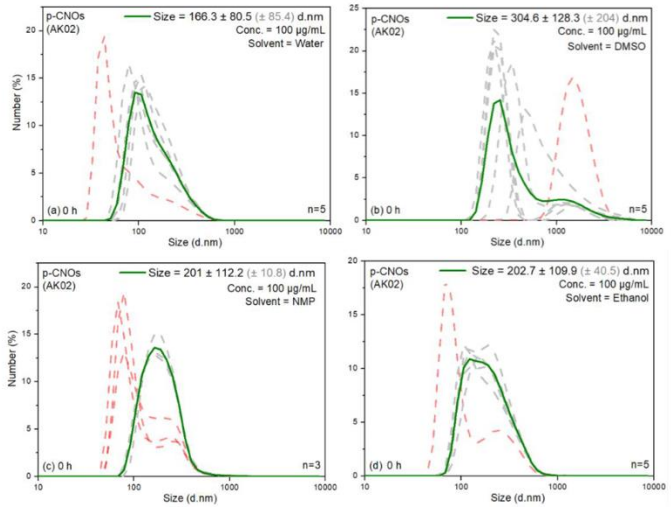
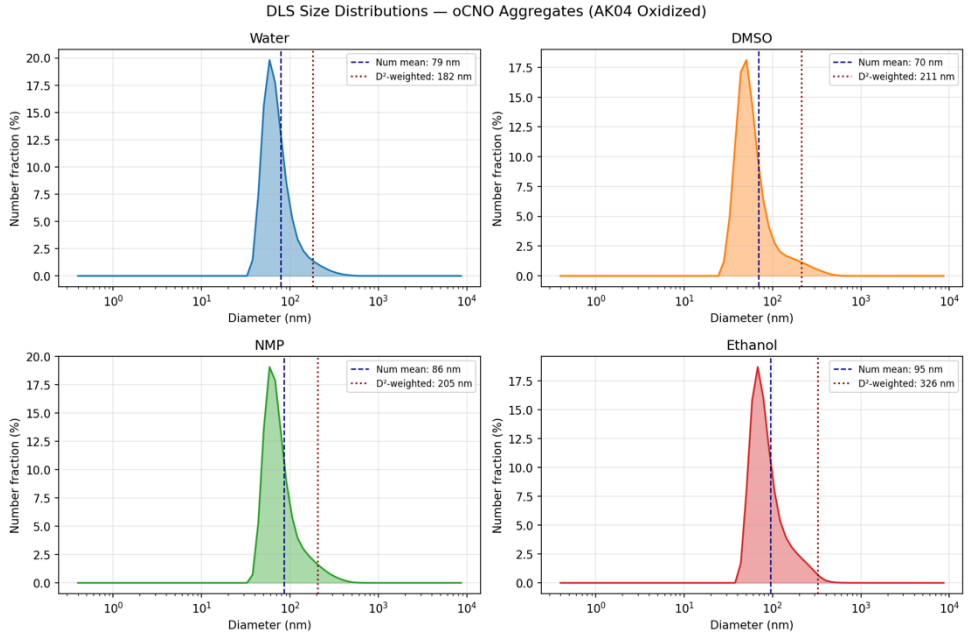


Figure 2 : DLS Size distribution of p-CNOs dispersed in water, DMSO, NMP and ethanol at 0 h. All solutions are of 100 µg/mL concentrations. The green curve shows the average size calculated from the grey dash curves. The faint red curves are neglected when average is calculated . The ± value given in gray alongside the standard deviation is the deviation between the curves used to calculate the total average size.



pCNO DLS

DLS can be converted to lognormal parameters or read as an exported distribution curve.

oCNO DLS

Oxidation changes solvation and aggregate state, so DLS must enter the optical model.

Fitting workflow: UV–Vis → aggregate f_V

A code-based route from experimental spectrum to a physically interpretable aggregate volume fraction.

1. Input spectrum → **2. Select medium** → **3. Add DLS** → **4. Fit f_V**

1. Input spectrum	2. Select medium	3. Add DLS	4. Fit f_V
UV–Vis CSV	Water / DMSO / NMP / Ethanol n,k	CSV distribution or Dg, σg	shape or amplitude window

What is actually fitted?

f_V changes two linked quantities:

- aggregate effective n,k from Maxwell–Garnett EMT
- number of hydrodynamic aggregates for a fixed CNO mass concentration

Example command

python utils/fv_fit.py

```
--exp-data expdata2/AK23_Oxi_Water_25.csv
--medium Water --cno-material f --oCNO
--dls-curve expdata2/DLS_AK04_Oxi_Water.csv
--fit-window 200:350
```

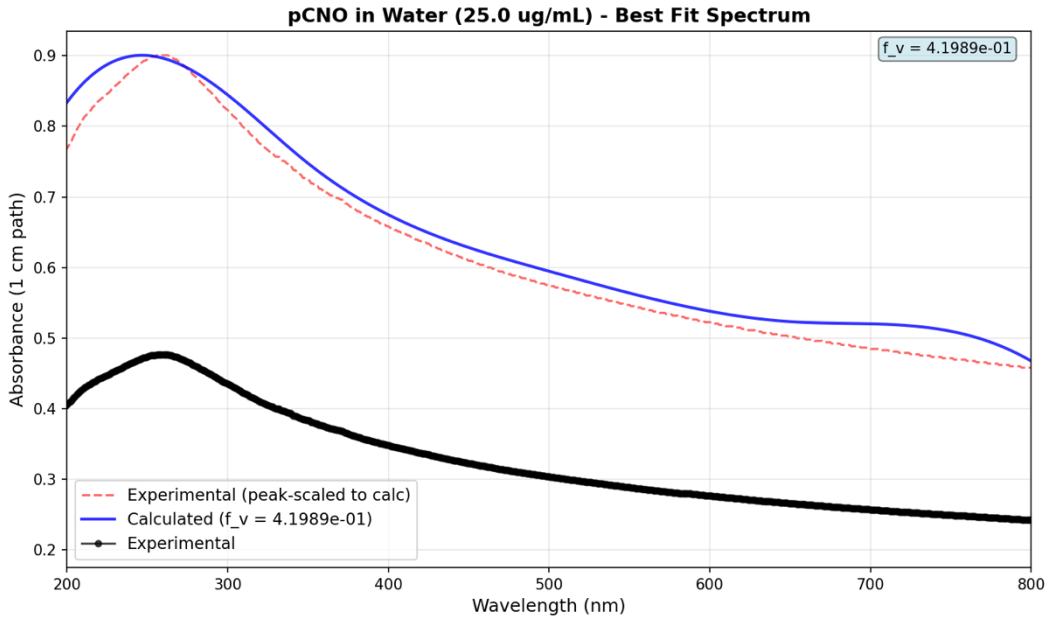
Output to discuss

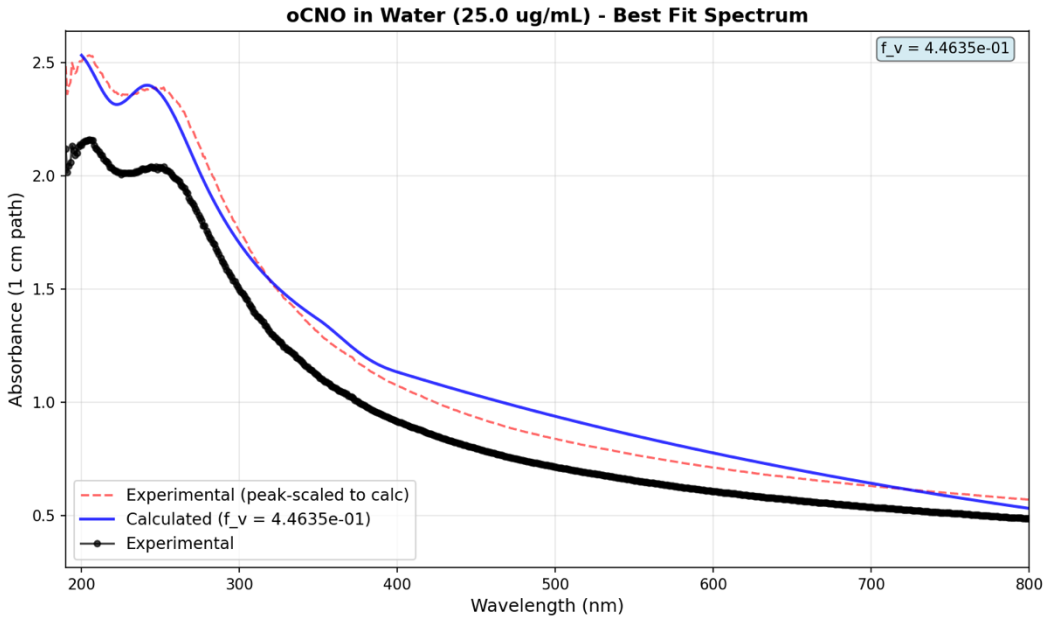
best f_V + peak match + linewidth + baseline residual

Then check whether the assumed solvent, DLS distribution and effective concentration are physically reasonable.

Case study: fitting Water spectra

pCNO and oCNO require different surface / aggregate interpretations





pCNO Water

model captures main UV feature; residual long-wavelength tail informs bg2/background choice

oCNO Water

additional surface absorption term helps reproduce the far-UV feature

Laser heating

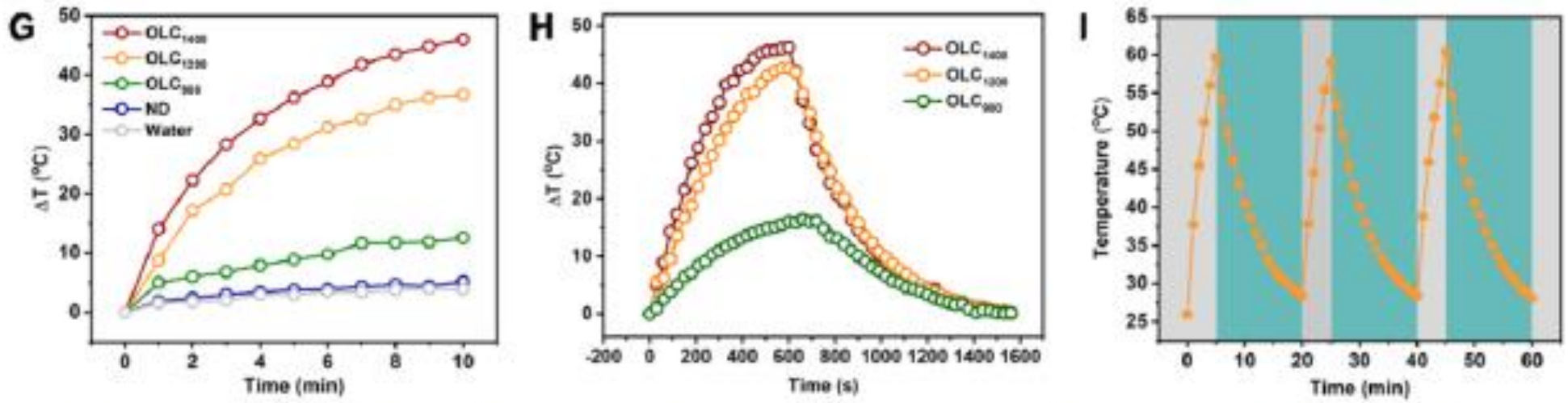


Figure 1. (A–D) TEM images of ND, OLC_{900}, OLC_{1200} and OLC_{1400}. (Scale bar: 2 nm) (E) Raman spectra and (F) of ND, OLC_{900}, OLC_{1200}, and OLC_{1400}. (G) Temperature change curves of different materials in 10 min (power density: 1.75 W/cm^2, concentration: 50 μg/mL). (H) Heating and cooling process of OLCs obtained at different temperatures (power density: 1.75 W/cm^2, concentration: 100 μg/mL). (I) Photothermal stability of OLC_{1400} in 3 heating–cooling cycles (power density: 1.75 W/cm^2, concentration: 100 μg/mL).

Laser Heating Model — Implementation

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From optical absorption to bulk temperature rise

1 Core equations

Absorbed power (Beer–Lambert)

$$P_{a\beta s} = I \cdot A_{\beta eam} \cdot (1 - 10^{-A808}) \cdot \eta$$

A_{808} = sample absorbance at 808 nm | η = photothermal conversion efficiency

Lumped 0-D heat balance

$$m\, C_p \cdot dT/dt = P_{a\beta s}(t) - h\, A_{expose} \mathcal{d}\, (T - T_{am\beta})$$

Heat gain from absorbed laser power balanced by convective heat loss.

2 Numerical update

Explicit Euler time stepping

$T_{n+1} = T_n + \Delta t \cdot [P_{a\beta s}(t_n) - hA_{expose}\mathcal{d}(T_n - T_{am\beta})] / (mC_p)$

Time step

$\Delta t = 1$ s
Sufficient for bulk water–sample scale heating curves.

Key interpretation

At the water–sample scale, temperature mainly follows average absorbed power.

Laser Heating Model — Parameters

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Default values and material cases used in the simulation

1 Default parameters

I at 808 nm	1.75 W cm^{-2}
h	80 W m^{-2} K^{-1}
$T_{am\beta}$	25 °C
water C_p	4.18 J g^{-1} K^{-1}

2 Material cases

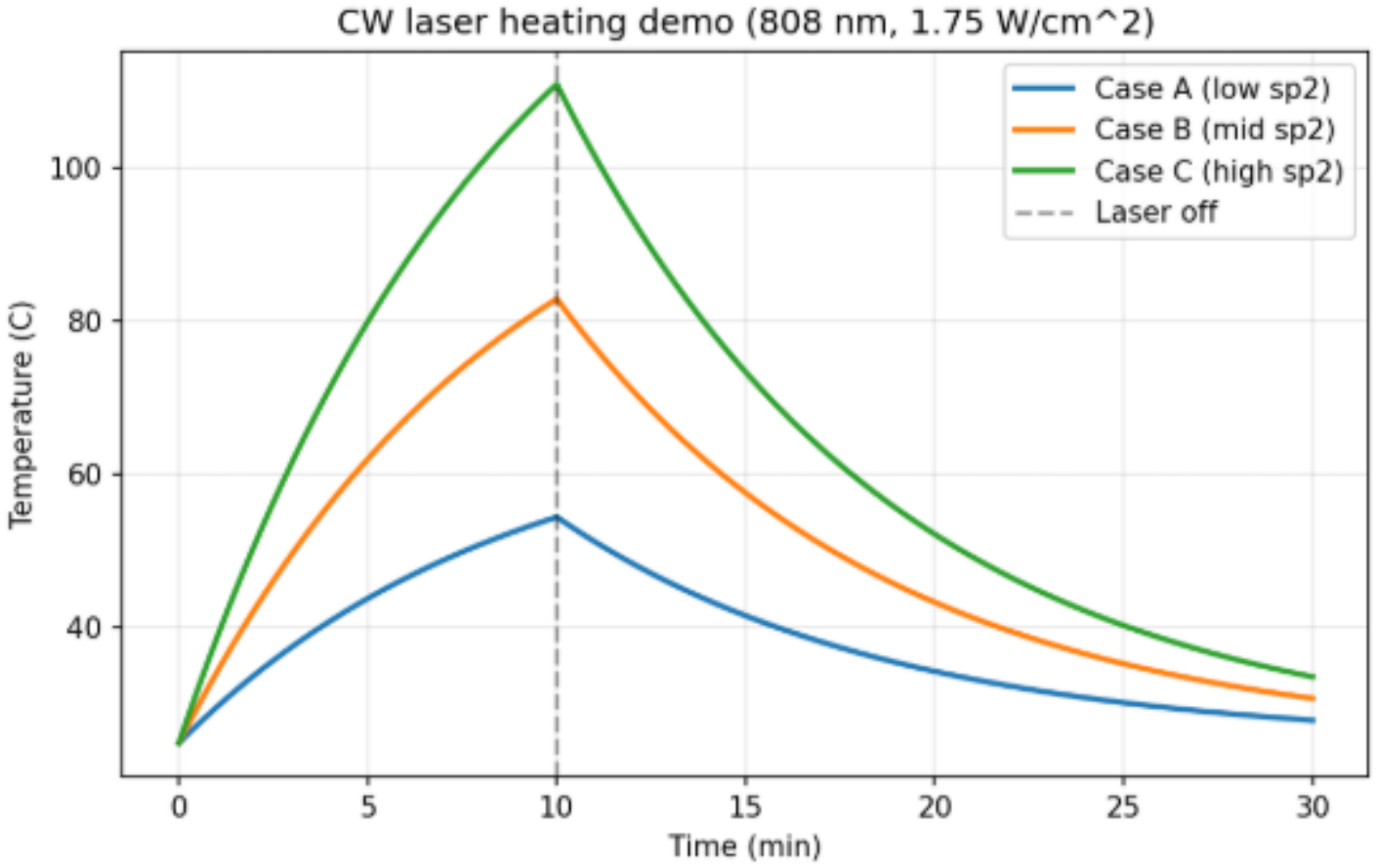
Varying sp^2 content, informed by literature photothermal conversion efficiency values:

Low sp^2	$A_{808} / \eta = 0.25 / 0.45$
Mid sp^2	$A_{808} / \eta = 0.45 / 0.60$
High sp^2	$A_{808} / \eta = 0.65 / 0.74$

Benchmark note

The high-sp^2 case matches the ~74% PCE benchmark from Feng et al. 2024.

CW heating model



python testcode/laser_heating_demo_cases.py

CW vs Pulsed Laser — Same Average Power

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Implemented in utils/laser_heating_comparison.py

1 Pulse definitions

$$E_{pulse} = P_{avg} / f_{rep}$$
$$P_{peak} = E_{pulse} / \tau_p$$
$$\text{Duty cycle} = \tau_p \cdot f_{rep}$$

2 Absorbed energy

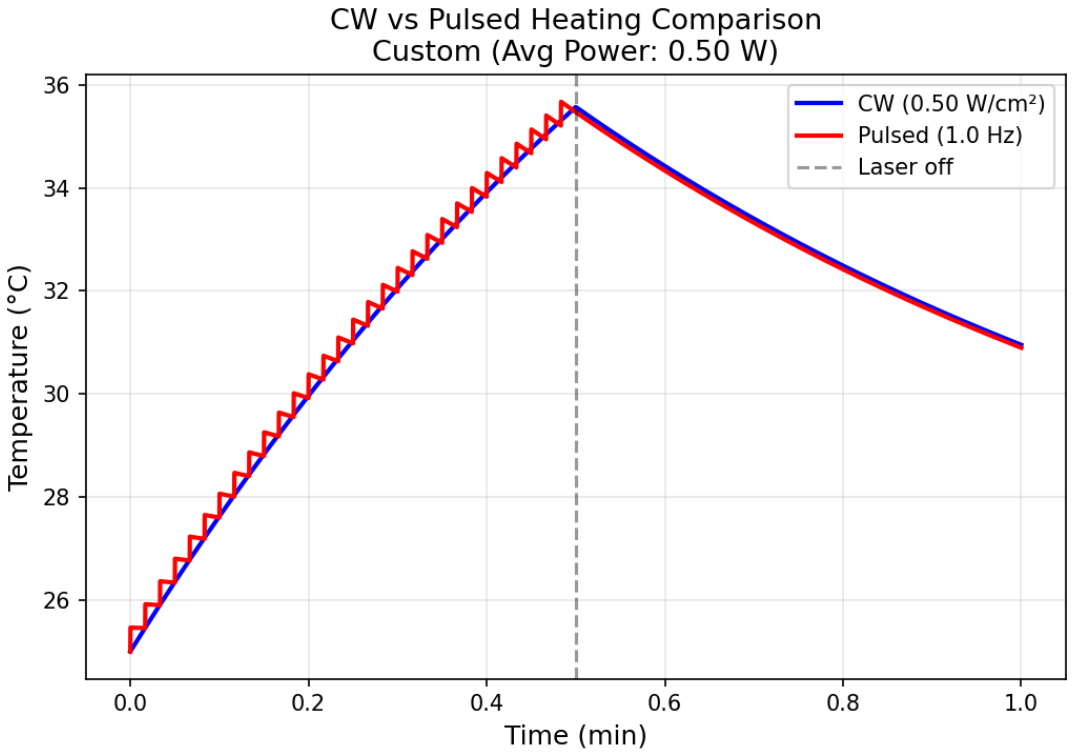
$$E_{abs,pulse} = E_{pulse} \cdot (1 - 10^{-A808}) \cdot \eta$$

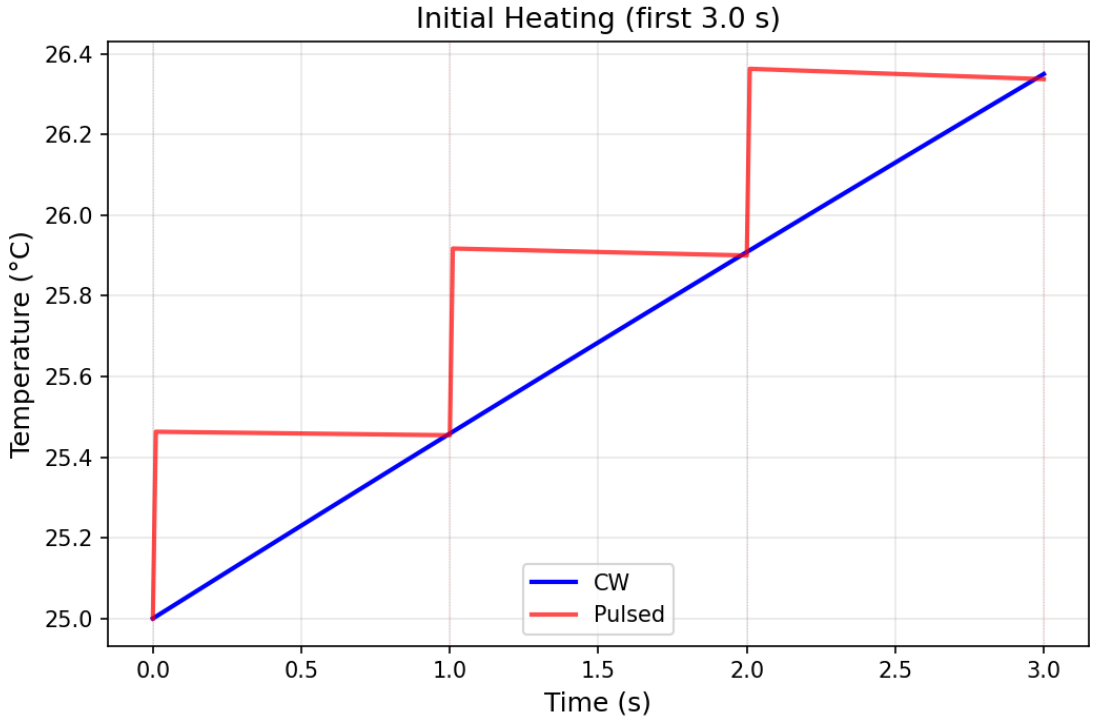
Heat loss remains continuous.

Interpretation With the same average absorbed power, pulsed input is thermally smoothed at the water–sample scale; the bulk temperature mainly follows average power.

Next step For true pulsed-laser nanothermal physics, couple optical absorption to local heat diffusion around CNOs and aggregates.

CW vs pulsed (10ms, 1Hz)

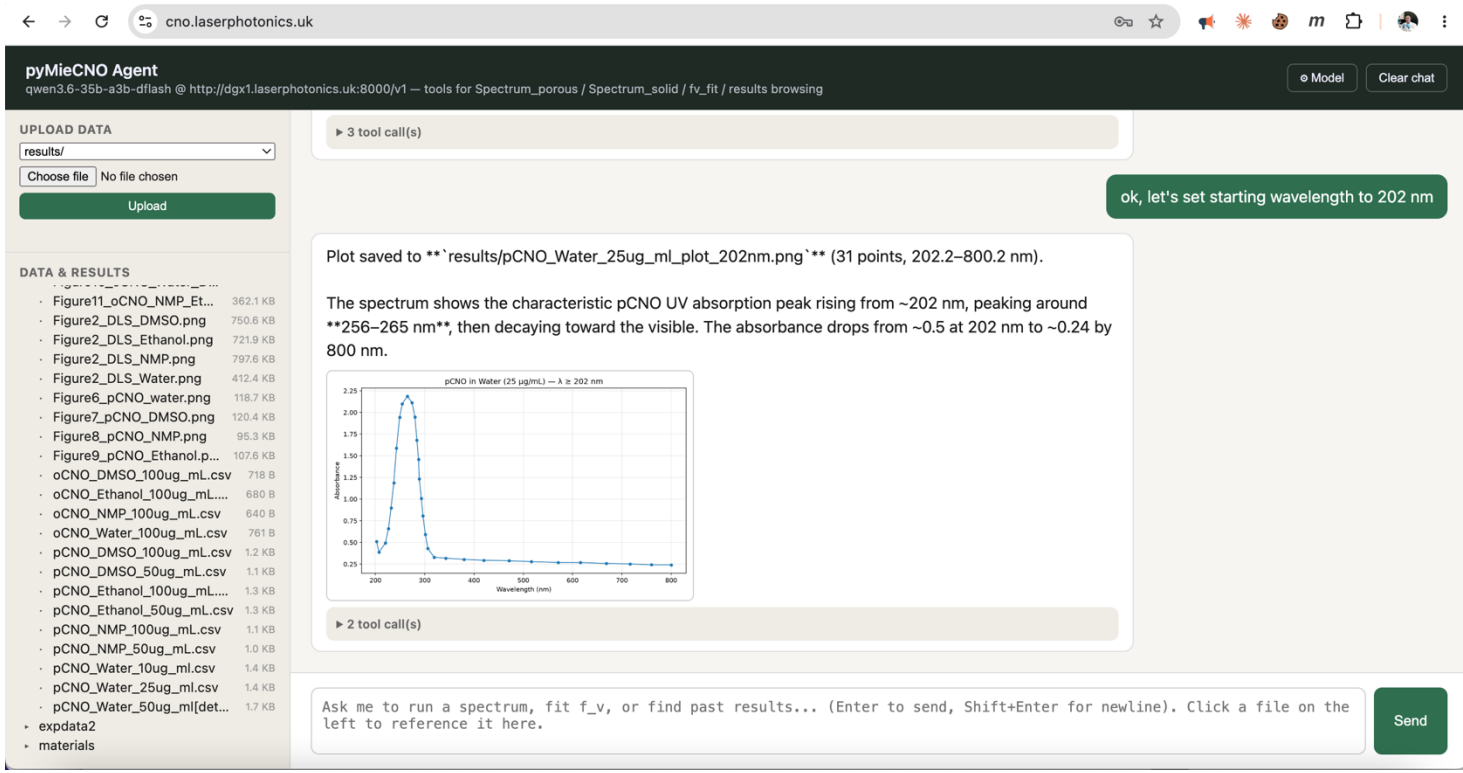




An AI Agent for CNO Modeling

- **Current:** Python command-line based

- **Accelerating the Workflow using AI agent:**
  - Webui
  - Natural lanaguge input
  - Backend LLM model



AI Agent Interface for CNO Modeling

A locally hosted LLM with tool-calling access to the same pyMieCNO scripts

1. Run Spectrum Calculations

Porous (Maxwell-Garnett EMT) and solid (Mie) aggregate spectra, on request, in natural language

✓ No CLI syntax to remember | ✓ Consistent defaults | ✓ Instant plots

Best for: quick what-if exploration during analysis

2. Fit Experimental Data

Volume-fraction (f_v) fitting to any UV-Vis spectrum via fv_fit, run as a background job

✓ Long fits (minutes) don't block the session | ✓ Live progress tracking

Best for: matching new samples without hand-tuning CLI flags

3. Browse, Explain & Analyze

Searches past results, summarizes CSVs, answers modelling questions, runs custom Python snippets

✓ Answers grounded in the project's own source/docs, not assumptions | ✓ Upload new data directly

Best for: onboarding collaborators, revisiting old fits, ad-hoc analysis

Runs on a self-hosted local LLM — no data leaves the lab

Live Demo

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- “Show me the single CNO particle absorption spectrum for water”
- “expdata2/AK02_pCNO_Water_25.csv, plot this and find peak”
- “What's the best CNO volume fraction fit we've found for oxidized CNO in Water?”

Github code at:

- https://github.com/ZengboJamesWang/pyMieCNO
- Support single and aggregates calculation
- Please contact z.wanng@bangor.ac.uk for access if needed.

Join our COST Action network bid

CARBON-X: AI-enabled standardisation and translation of zero-dimensional carbon nanomaterials

Open invitation

We are building a European network linking carbon nanomaterials, photothermal therapy and agentic AI-enabled standardisation.

Especially welcome: researchers and early-career colleagues from COST Inclusiveness Target Countries (ITC).

Please speak to me after the session if you work on carbon materials, AI/autonomous lab tools, biology or nanomedicine.

Key focus areas

Standardisation

Comparable synthesis, characterisation and reporting protocols for 0D carbon nanoparticles.

Translation

Move from optical models and in-vitro data towards reproducible nanomedicine use cases.

AI-enabled workflow

Use agentic AI/autonomous-lab tools to capture data, guide experiments and improve reproducibility.

Training & mobility

Shared protocols, short visits, workshops and cross-sector collaboration across Europe.