Nanoscattering Software

February to July 2022

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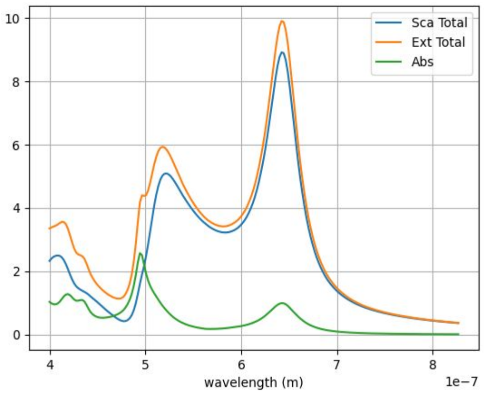
Nanomade Team

Working Principle

Mie Theorie



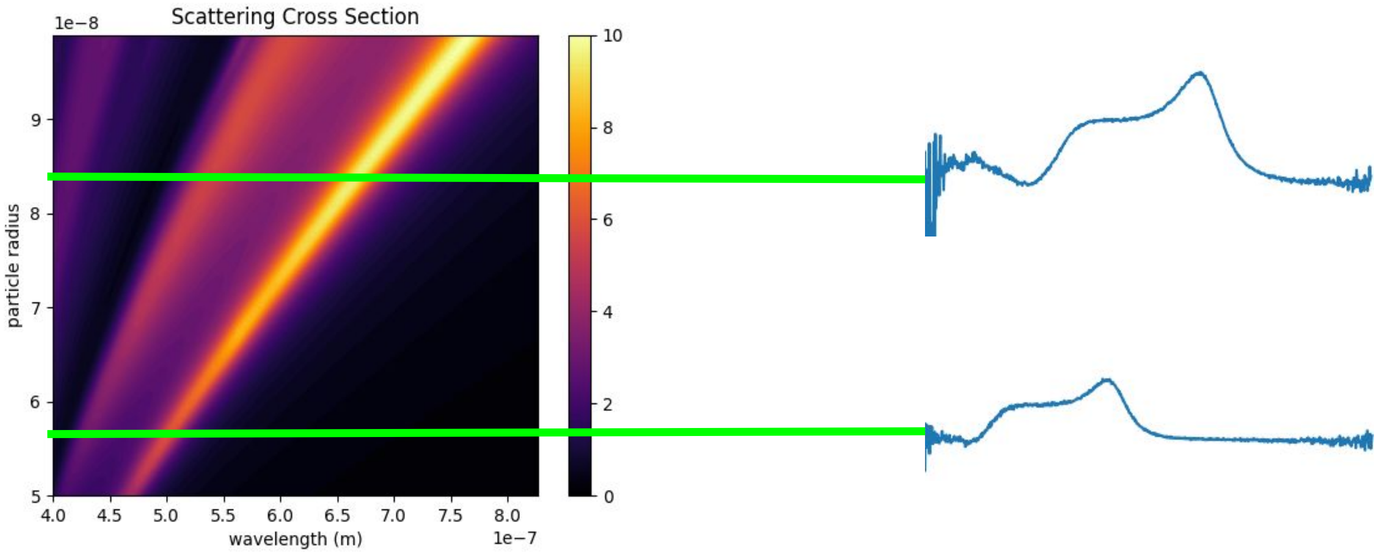
Unique Particle Size (80 nm)

Experimental Spectrum (Optical Microscope)

Working Principle

Comparison with each computed radius

Surface



Set of Radius (50 nm to 100 nm)

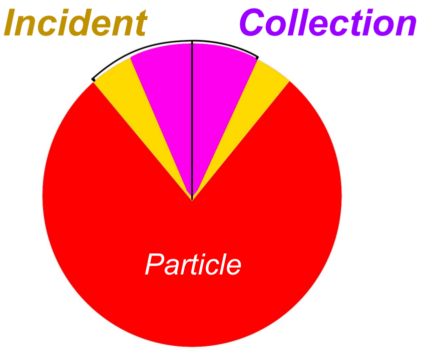
Compute Surface

Main Formula for simulation:

$$W_s = \frac{1}{2k\omega\mu}\left[\int_{\phi_1}^{\phi_2} \cos^2\phi \, d\phi \int_{\theta_1}^{\theta 2} \Re\left\{\sum_{n=1}^{\infty} E_n(i a_n \xi_n' \tau_n - b_n \xi_n \pi_n)\left(\sum_{n=1}^{\infty} E_n(i b_n \xi_n' \pi_n - a_n \xi_n \tau_n)\right)^*\right\} \sin\theta \, d\theta \right.$$
$$\left. - \int_{\phi_1}^{\phi_2} \sin^2\phi \, d\phi \int_{\theta_1}^{\theta 2} \Re\left\{\sum_{n=1}^{\infty} E_n(b_n \xi_n \tau_n - i a_n \xi_n' \pi_n)\left(\sum_{n=1}^{\infty} E_n(i b_n \xi_n' \tau_n - a_n \xi_n \pi_n)\right)^*\right\} \sin\theta \, d\theta \right]$$

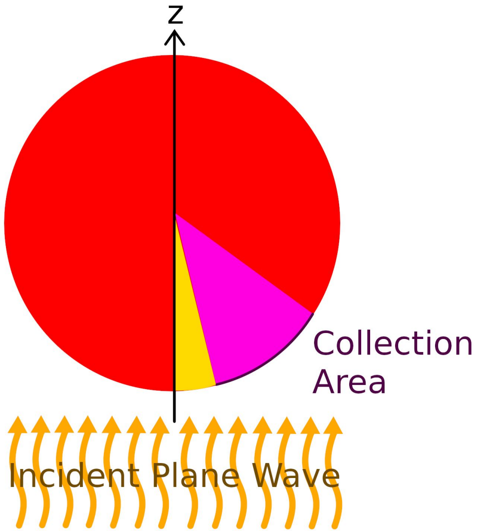
ϕ and θ represent the spherical coordinates where the scattered light is collected

Experimental Collection Shape:



Compute Surface

Wished Shape Applied for the Simulation:



Note: Due to the small size (nano scaled) of the particle, the shape of the incident light doesn't matter. Only the collection shape is important here.

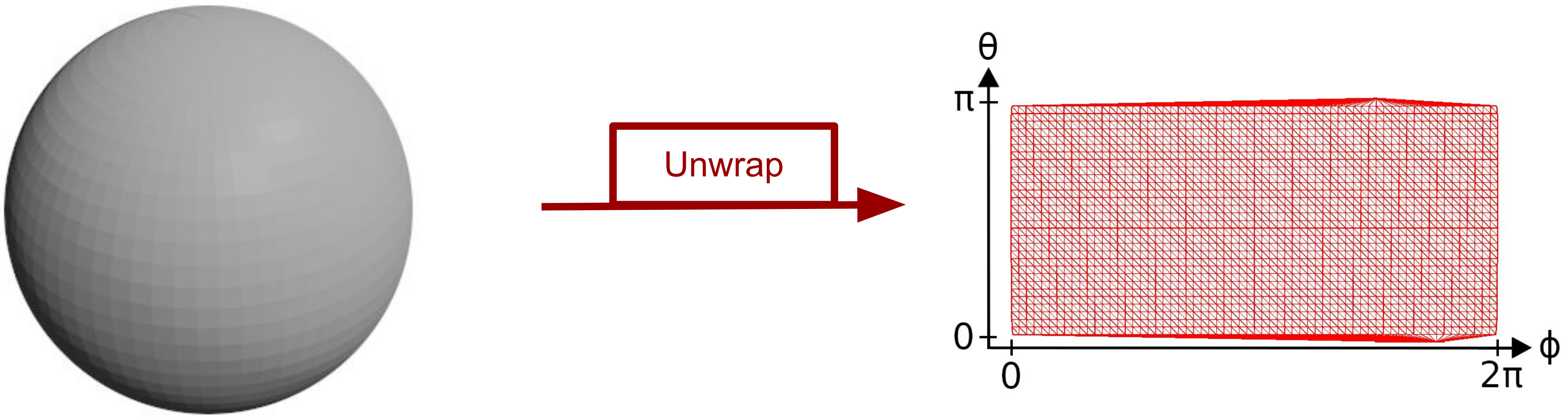
Problem:

Integration by variables (ϕ and θ) doesn't support these kinds of shape: it's mathematically impossible to parametrize these variables in order to obtain this specific *disk* shape.

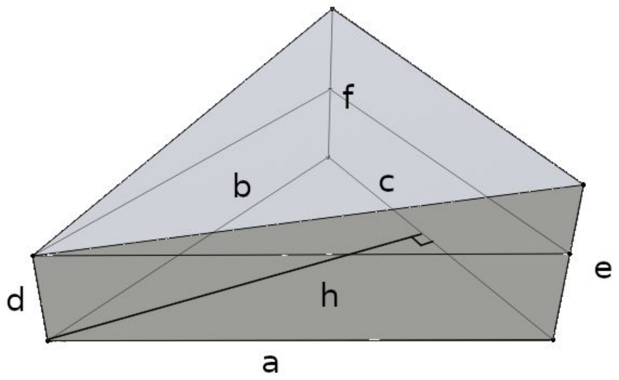
Solution:

Numerical integration being equivalent to a summation, we compute each value of the *main* equation at (ϕ, θ) then sum all of them in the wished shape.

Compute Surface



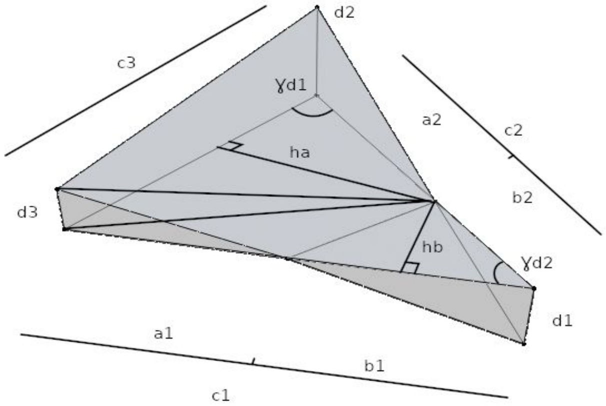
Compute Surface



$$h = \sin(\frac{a^2 + c^2 - b^2}{2ac})$$

$$V_1 = \frac{1}{2}cahd$$

$$V_2 = \frac{1}{3} \times \frac{(f+e)c}{2} \times h$$



$$a_1 = \frac{c_1}{1 + d_1/d_3} \quad b_1 = \frac{d_1 a_1}{d_3} \quad a_2 = \frac{c_2}{1 + d_1/d_2} \quad b_2 = \frac{d_1 a_2}{d_2}$$

$$h_a = a_2 \sin(\gamma_{d_2}) \quad h_b = b_2 \sin(\gamma_{d_1})$$

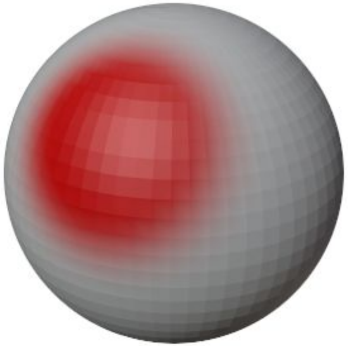
$$\gamma_{d_1} = \arccos(\frac{c_1^2 + c_2^2 - c_3^2}{2c_1c_2}) \quad \gamma_{d_2} = \arccos(\frac{c_2^2 + c_3^2 - c_1^2}{2c_2c_3})$$

$$V_1 = \frac{d_1 b_1}{2} \times h_b \times \frac{1}{3} \quad V_2 = \frac{d_3 a_1}{2} \times h_b \times \frac{1}{3}$$

$$V_3 = \frac{(d_2 + d_3)c_3}{2} \times h_a \times \frac{1}{3}$$

$$V_{Total} = \sum V_i$$

Selection
(by color)

Choose precision (blender) →  → Export “.ply”

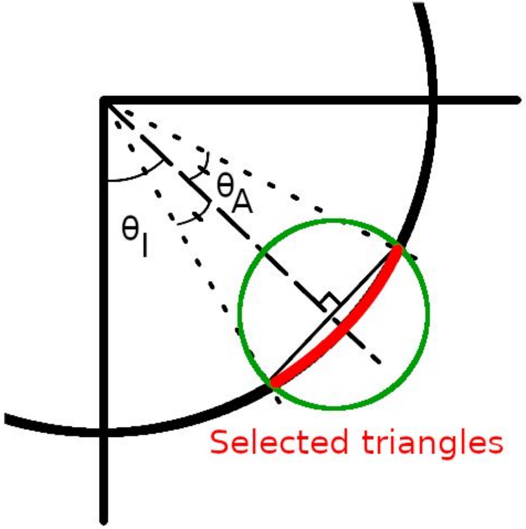
- *particle-32x16-low.blend*
- *particle-64x32-medium.blend*
- *particle-128x64-high.blend*

Colorize the wished surface

Selection (by angle)

Choose precision

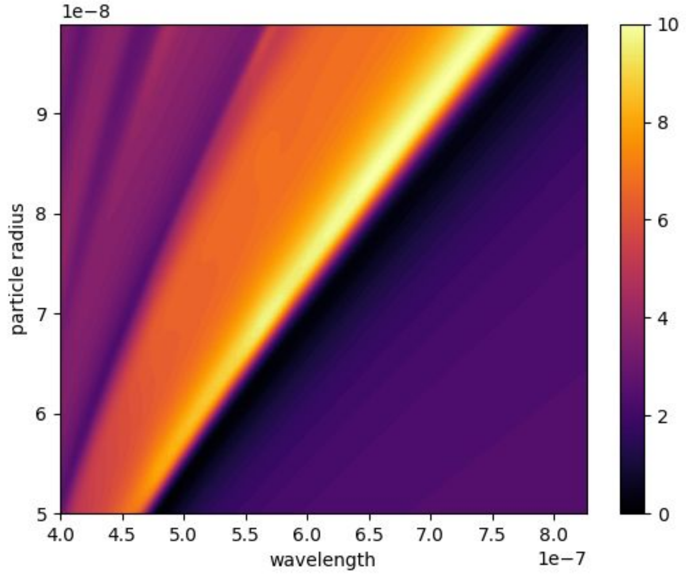
- *whole-low.ply*
- *whole-medium.ply*
- *whole-high.ply*



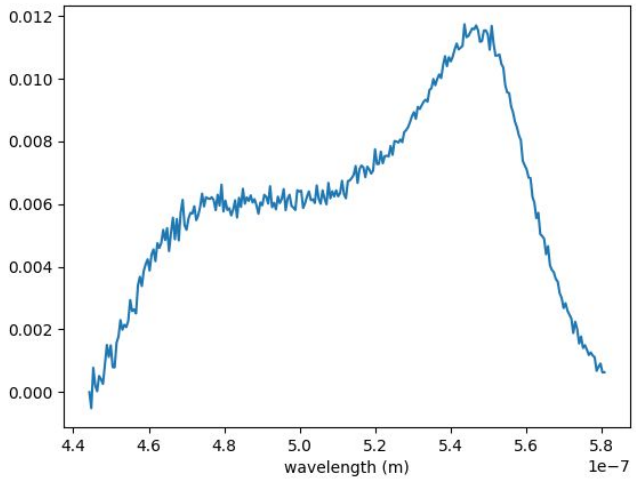
Select proper angles (inside the software)

Find Radius

Challenge: Find the best theoretical spectrum fitting the experimental one



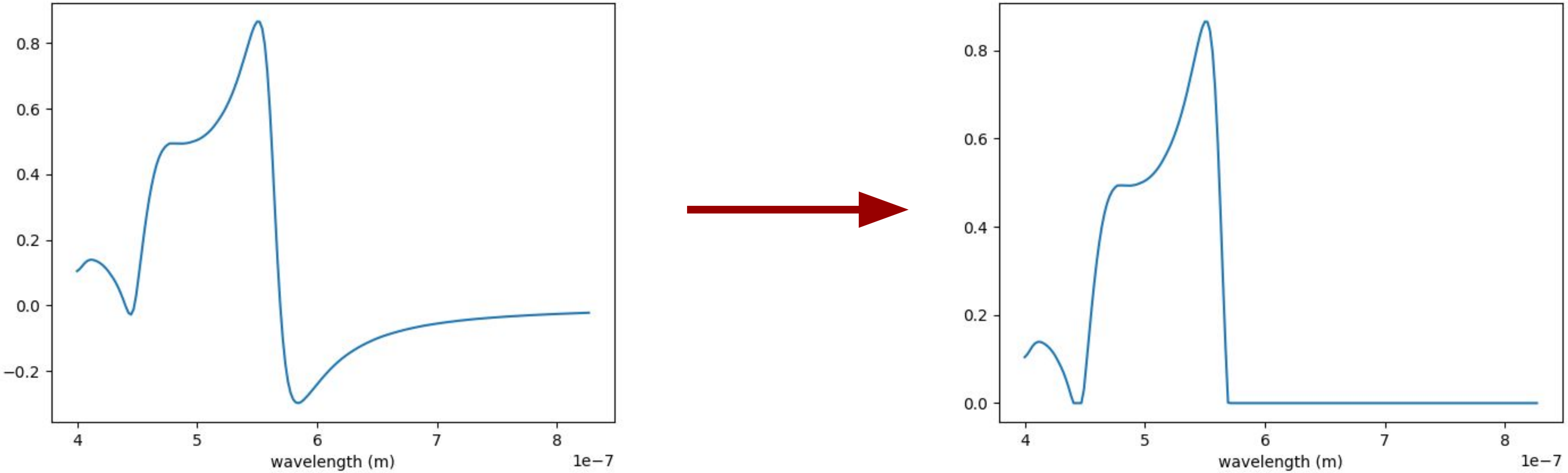
n_a = 0.2 x π and n_i = 0.25 x π with “whole-high.ply”



67 nm (radius) according to the AFM measurements

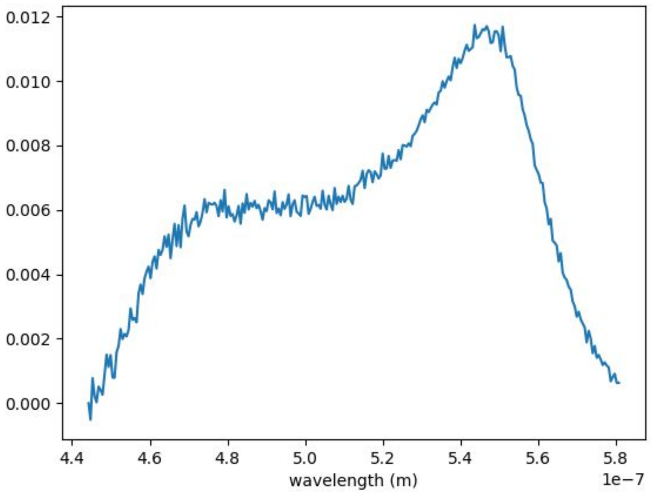
Find Radius

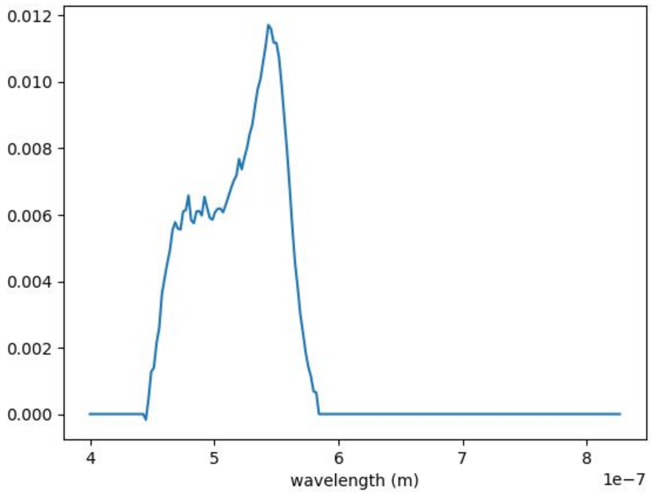
Transformation on **each** theoretical spectrum: remove negative values



Find Radius

Transformation on **the** experimental spectrum: redistribute values in the same range of wavelength

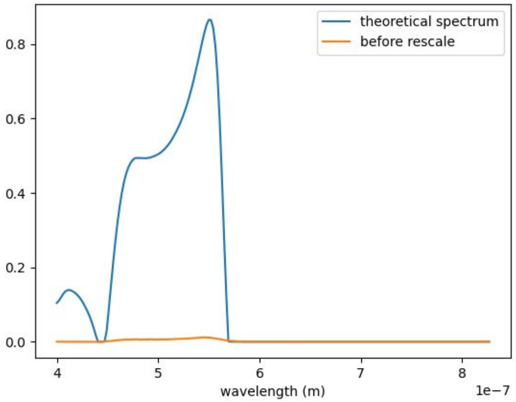


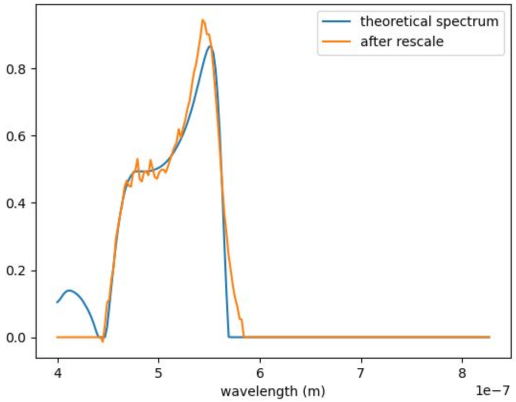


Find Radius

Rescale by area: g(x) = experimental spectrum ; f(x) = theoretical spectrum

$$A \times \int_{-\infty}^{+\infty} g(x)dx = \int_{-\infty}^{+\infty} f(x)dx \quad \longrightarrow \quad A = \frac{\int_{-\infty}^{+\infty} f(x)dx}{\int_{-\infty}^{+\infty} g(x)dx}$$

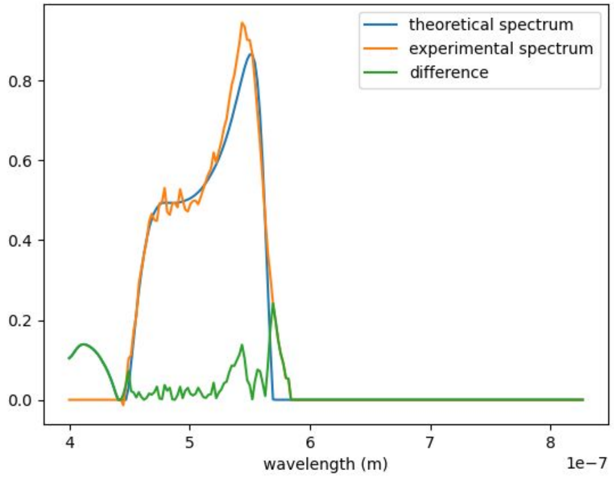




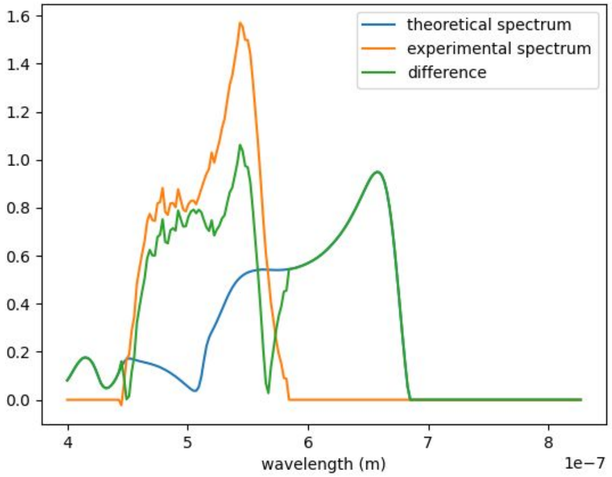
Find Radius

Compute the absolute difference in order to avoid negative compensations after integration

Best matching



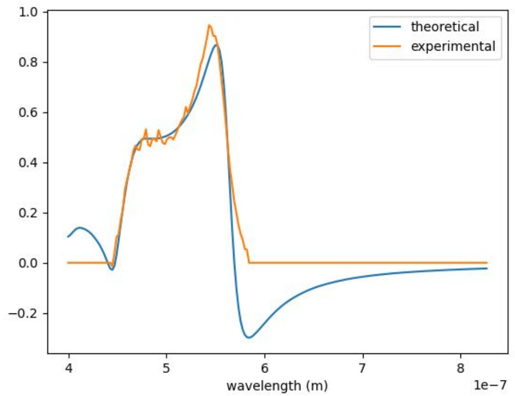
Worst matching

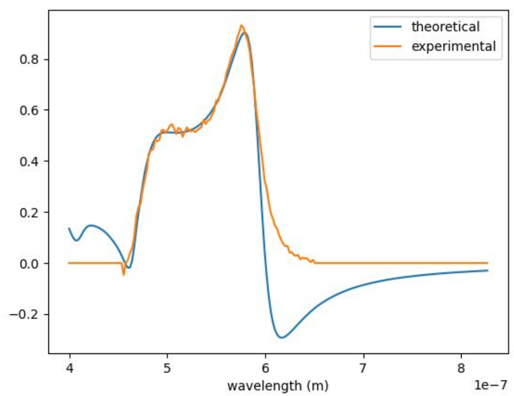


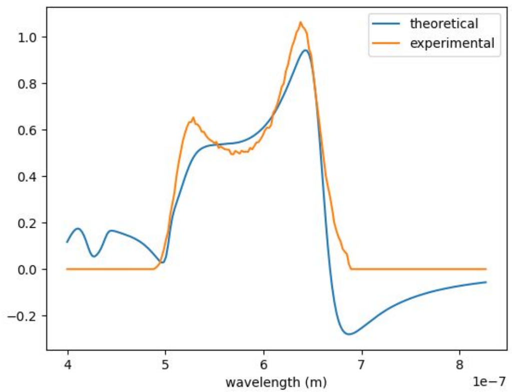
We keep the lowest value of the area described by the ***green curve****.*

Find Radius

Some examples…







AFM radius: 67 nm
Software: 66.8 nm

AFM radius: 72 nm
Software: 71.7 nm

AFM radius: 82 nm
Software: 82.1 nm

THE END