# Optical properties of Martian dust – II. Modeling

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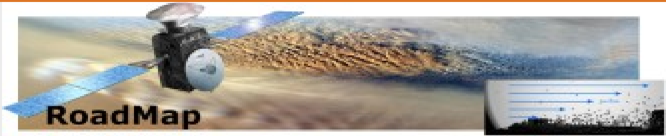
RoadMap: Dust on Mars Workshop
19.-21.9.2023

This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 101004052





# About me

- 2021: PhD in astrophysics at the University of Helsinki

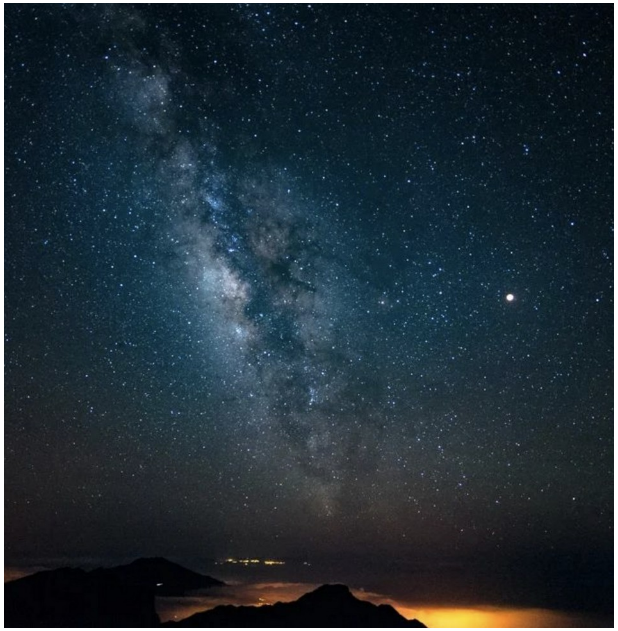
  - Specialization in light scattering: modeling, experiments, and observational astronomy

  - 2019-2021: Support astronomer at the Nordic Optical Telescope, La Palma, Spain

- 2021 →: Instituto de Astrofisica de Andalucia, Granada, Spain

  - Scientist in the RoadMap-project

  - Optical properties retrieval for Martian dust



Lunar eclipse, May 16th 2022, La Palma, Spain

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# Outline

## PART I: Theory

- Introduction to RoadMap
- Background: Scattering theory

## PART II: Modeling

- Modeling
- Samples
- Optical constants retrieval
- Scattering properties
- Summary

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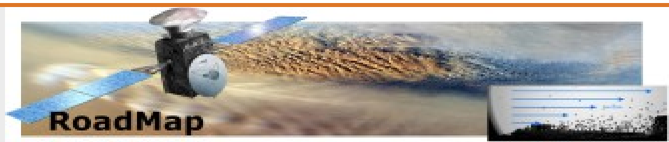

# PART I: Theory

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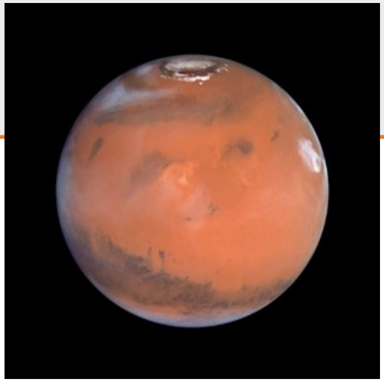
# Introduction to RoadMap



- RoadMap: ROle and impAct of Dust and clouds in the Martian AtmosPhere

  - Laboratory measurements and models to better describe Martian dust and clouds

  - Aim: database of scattering properties for Martian dust

- Optical constants, the complex refractive indices ($m=n+ik$), are needed in light scattering and radiative transfer models

  - The real part, *n*, describes the ratio of the speed of light in a vacuum to the phase velocity of light in the material

  - The imaginary part, *k*, describes the absorption of light inside the material

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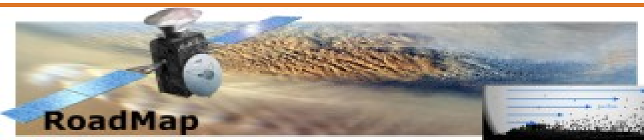


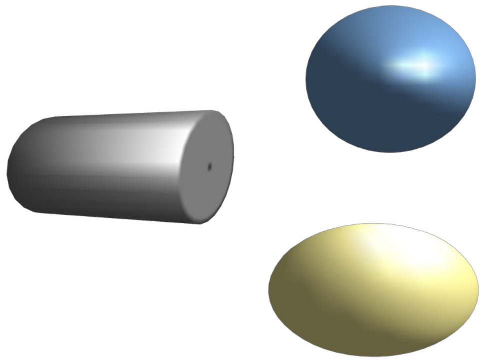
# Introduction to RoadMap

- Limitations on optical constant retrievals based on observations

  - multiple free parameters

  - simplified particle shapes: spheres, spheroids, cylinders

  - no direct particle size distribution measurements



- Experimental data needed to characterize the samples well

  - constraints on particle sizes and shapes → the only free parameter is the complex refractive index

  - combined with a model based on advanced numerical techniques

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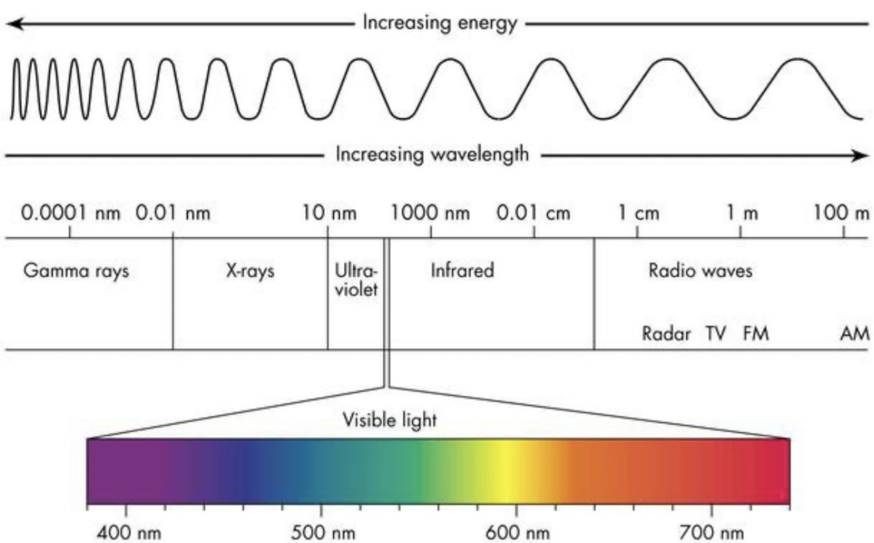
# Background: Scattering theory

- **Photometry**: measures the intensity of the object's electromagnetic radiation
- **Polarimetry**: study of the polarization of light
- **Spectroscopy**: how much electromagnetic radiation is scattered, absorbed, or emitted by the object at different wavelengths




cyberphysics.com.uk

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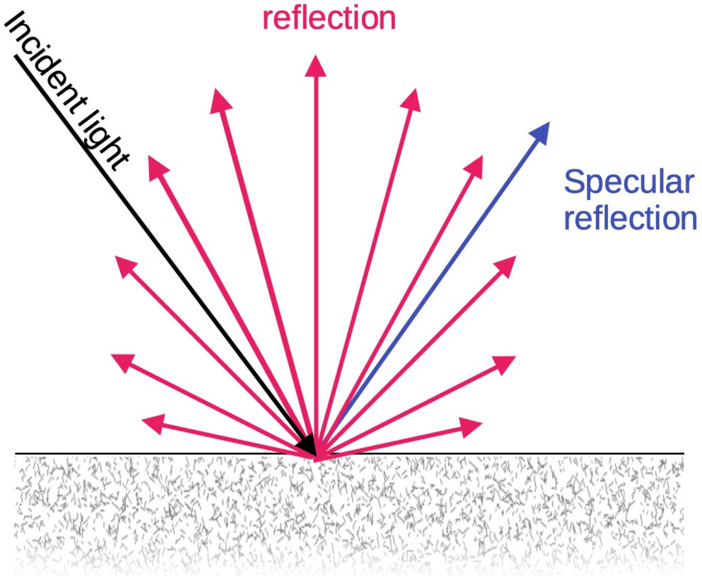
# Background: Scattering theory

## Spectroscopy

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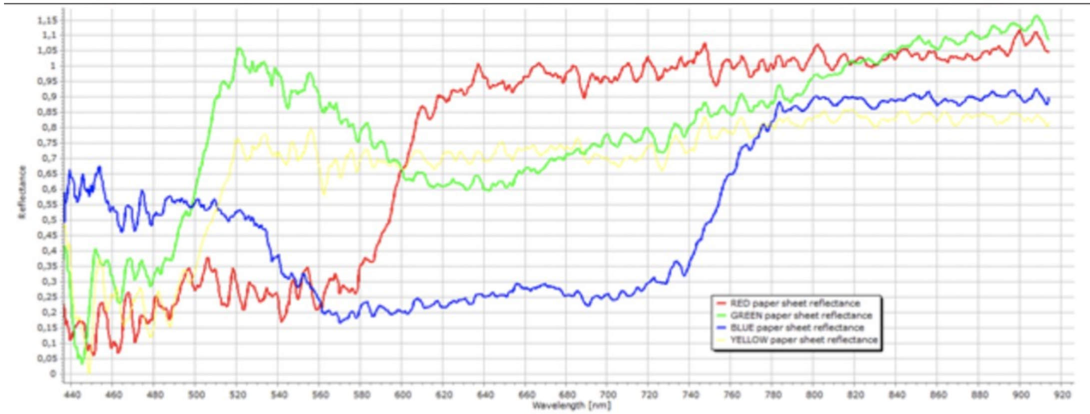


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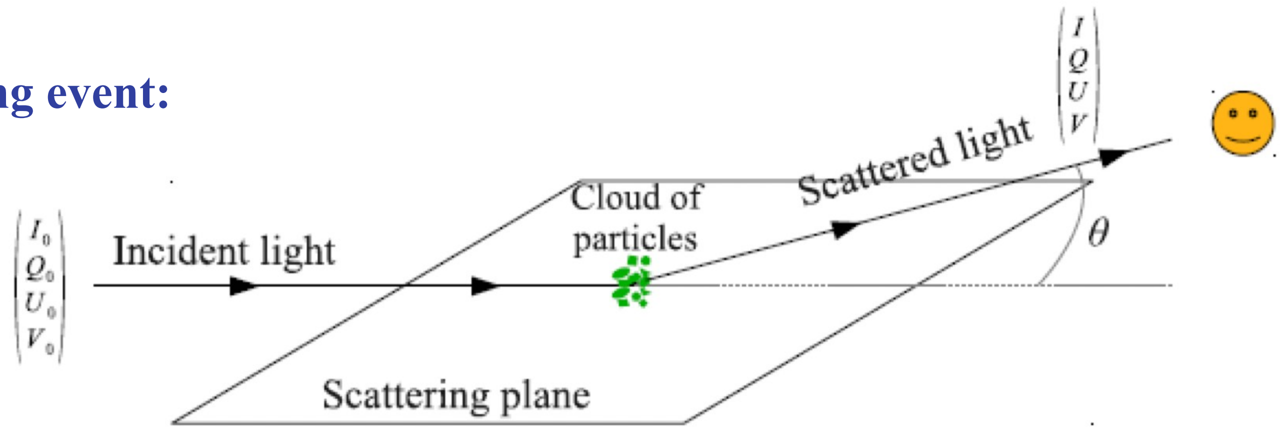
# Background: Scattering theory

**Scattering event:**




**Light characterized by the Stokes parameters**

$$\begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} = \frac{\lambda^2}{4\pi^2 R^2} \begin{pmatrix} F_{11} & F_{12} & F_{13} & F_{14} \\ F_{21} & F_{22} & F_{23} & F_{24} \\ F_{31} & F_{32} & F_{33} & F_{34} \\ F_{41} & F_{42} & F_{43} & F_{44} \end{pmatrix} \begin{pmatrix} I_0 \\ Q_0 \\ U_0 \\ V_0 \end{pmatrix}$$

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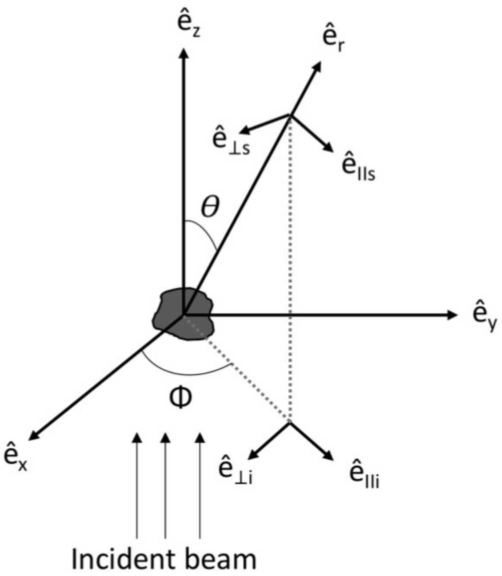
# Background: Scattering theory




- A scattering event can change the state of the incident light
  – The change is fully described by a 4x4 Mueller matrix, the so called **scattering matrix** F
  – F is a function of the scattering angle $\theta$ or the phase angle $\alpha = \pi - \theta$

- After a light beam interacts with an object, part of it can either scatter or be absorbed
  – Multiple factors affect the amount of scattering and absorption: **size** and **shape** of the object, **optical properties** (such as the complex refractive index), **porosity**, **particle orientation**, and the **wavelength** of the incident light

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# Background: Scattering theory

Phase function

Degree of linear polarization (DLP) = -F12/F11

Intensity

Lin. Pol.

Circular Pol.

$$\begin{pmatrix} I \\ Q \\ U \\ V \end{pmatrix} \propto \begin{pmatrix} F_{11} & F_{12} & F_{13} & F_{14} \\ F_{21} & F_{22} & F_{23} & F_{24} \\ F_{31} & F_{32} & F_{33} & F_{34} \\ F_{41} & F_{42} & F_{43} & F_{44} \end{pmatrix} \begin{pmatrix} I_0 \\ Q_0 \\ U_0 \\ V_0 \end{pmatrix}$$

Depolarization ratio

$$\delta_L = \frac{1 - F_{22}/F_{11}}{1 + 2F_{12}/F_{11} + F_{22}/F_{11}}$$

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# Background: Scattering theory

- The physical size of an object can be defined using a **size parameter**

$$x = \frac{2\pi a}{\lambda}$$

| Rayleigh | Resonance/Mie | Geometric Optics |
|---|---|---|
| $r \ll \lambda$ | $r \approx \lambda$ | $r \gg \lambda$ |

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# Background: Scattering theory

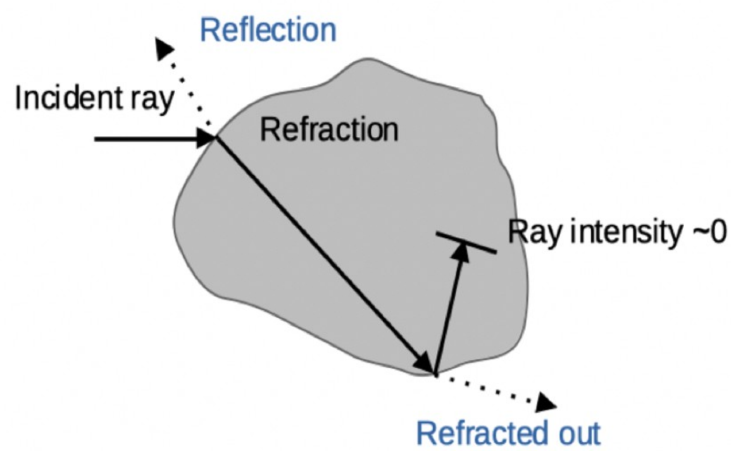
Light scattering by particles that are larger than the wavelength of the incident light can be solved with the help of ray optics

The 4x4 phase matrix **P** is given by: $\mathbf{P} = 4\pi\mathbf{F}/k^2\sigma_{sca}$

$\sigma_{sca}$ = scattering cross-section (the total scattered power). It can be divided into a ray-tracing part and a forward diffraction part

$\sigma_{sca} = \sigma_{sca}^{RT} + \sigma_{sca}^{D}$

The single-scattering albedo $\omega$ is $\sigma_{sca}/\sigma_{ext}$

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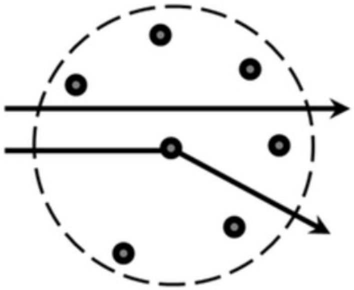
# Background: Scattering theory

- Single scattering vs. multiple scattering

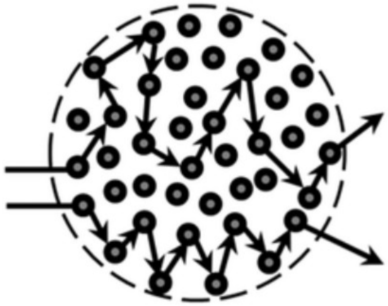
**Single scattering**

- Total Field = Σ *single fields*



**Multiple scattering**

- Radiative transfer equation



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# PART II: Modeling

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# Modeling: the general idea

## 1. Optical constants, *m*, retrieval

- Using advanced numerical methods (in geometric optics) and the measured reflectance spectrum of Martian dust analog samples

  - narrow size distributions needed for geometric optics!

- *m* is a parameter that depends on the material, not on the particle shapes or sizes

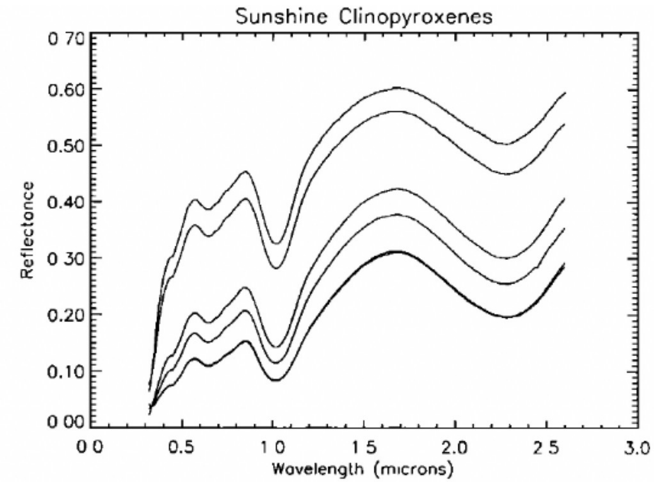
- measured reflectance spectrum depends on:

  - particle size (smaller particles show higher reflectance)

  - particle shape

  - m

  → important to use accurate particle sizes and shapes for the optical constants retrieval




Lucey 1998

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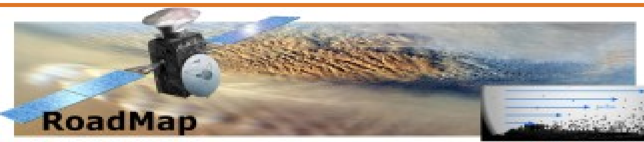

# Modeling: the general idea

**2. Validation of the retrieved optical constants**

- Use the derived *m* to reproduce the observed spectrum of Martian regolith

**3. Retrieval of scattering properties from the measured scattering matrices**

- Full scattering matrix **F** measured for all of the samples at 488 nm and 640 nm for L, M, and S size distributions

- Use the derived *m* together with a scattering database to obtain scattering properties such as the **single-scattering albedo**, **extinction efficiency**, and **asymmetry factor**

- Fine-tune the retrieved *m*

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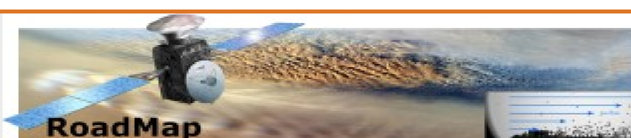

# Samples: starting point

- JSC Mars-1 (Allen et al. 1997): larger than 200 µm

| JSC Mars-1 simulant | MMS-2 simulant |
|---|---|
| Glassy, altered volcanic ash from Pu'u Nene, Hawaii | Iron-rich basalt mined from the Western Mojave desert |
| Amorphous palagonite, crystallites of plagioclase and magnetite | Crystalline plagioclase, pyroxene, magnetite, and hematite, with trace ilmenite and olivine |
| Glassy in texture | Crystalline in texture |

- Enhanced Mojave Mars Simulant (MMS-2, The Martian Garden): larger than 200 µm

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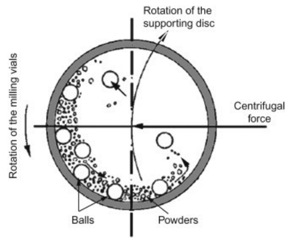
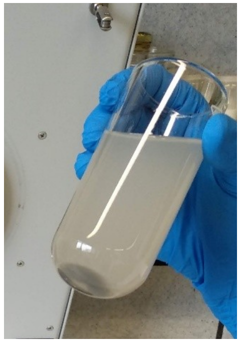
# Samples: processing

CSIC ICV
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS
INSTITUTO DE CERÁMICA Y VIDRIO (ICV)




MILLING

Crushed powders



SIEVING, DECANTATION (gravitational separation) CENTRIFUGATION

N dust fractions
**narrow size distributions**

Attrition mill


Grinding balls

Powder sieves (500 – 5 μm)

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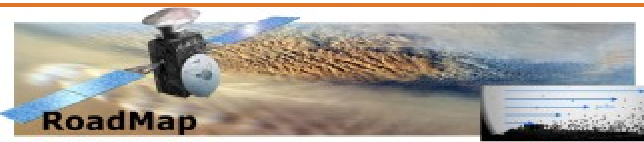


# Samples: processing

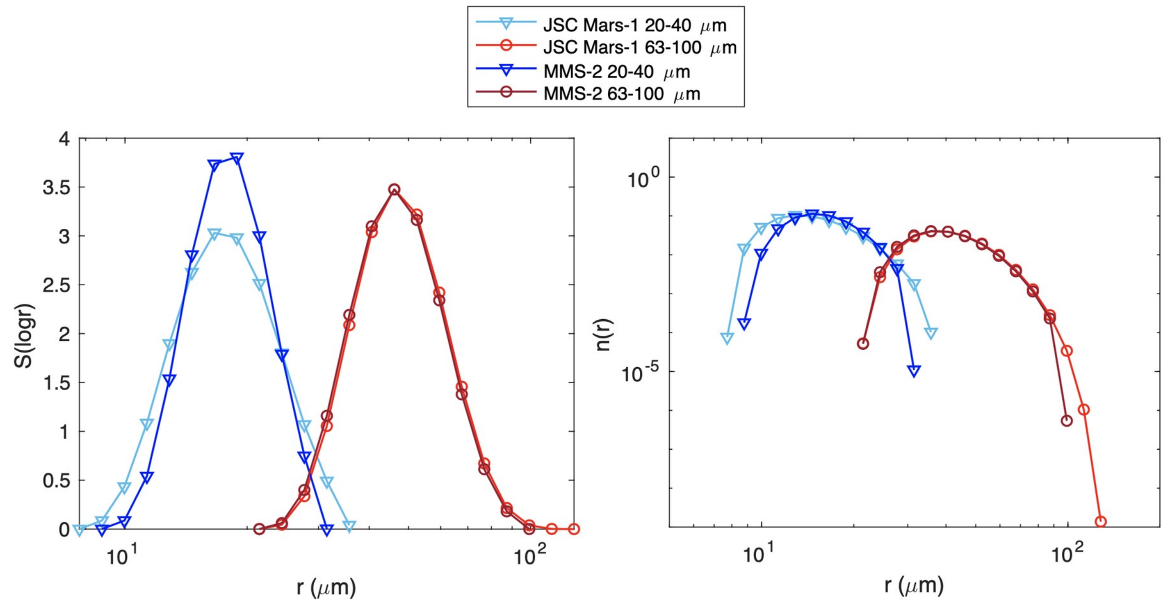
1. Larger than 200 microns (experimentally centered at D[4;3]: 275 μm)
2. Between 100 and 63 microns (centered at D[4;3]: 105 μm)
3. Between 40 and 20 microns (centered at D[4;3]: 40 μm)

- JSC Mars-1 63-100 μm

- JSC Mars-1 20-40 μm

- MMS-2 63-100 μm

- MMS-2 20-40 μm

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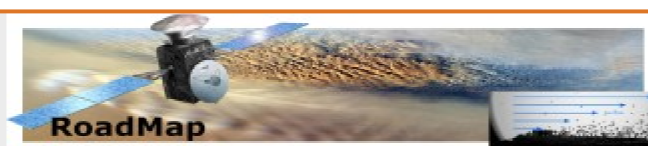
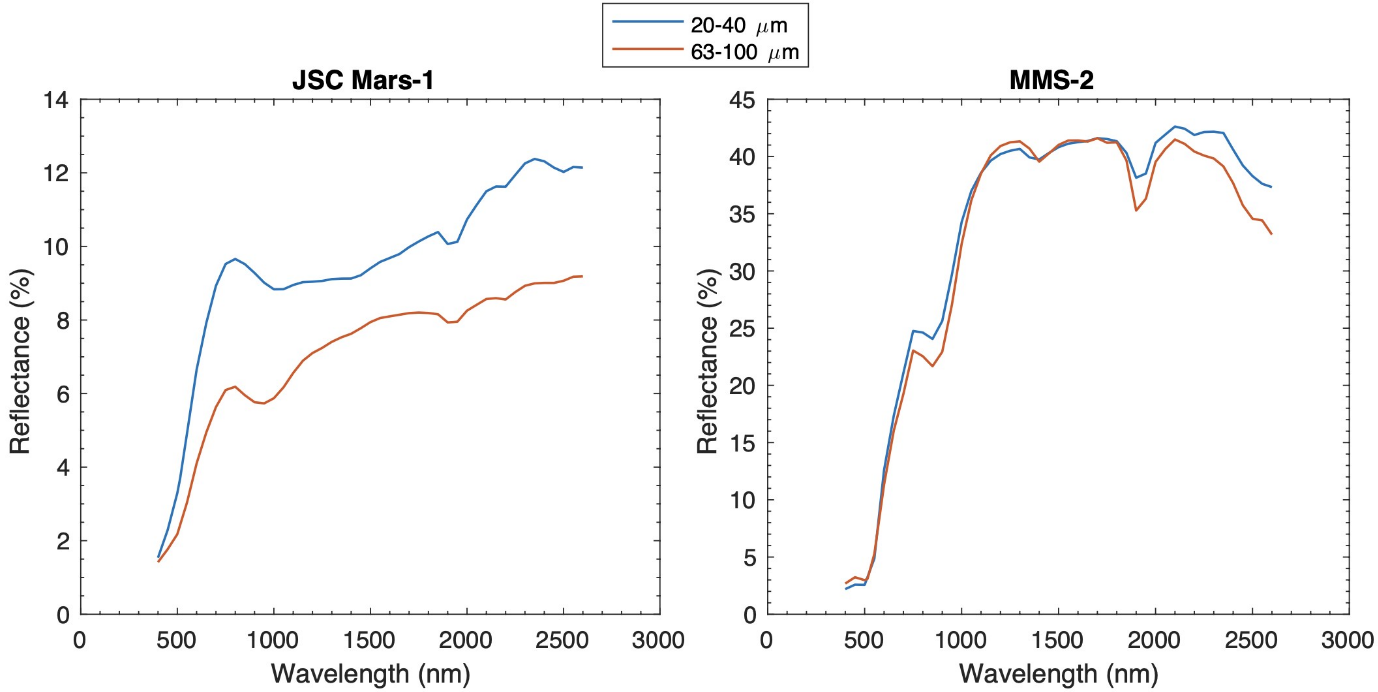


# Samples: spectral measurements

- Diffuse reflectance spectra measured at Centro de Instrumentación Científica, University of Granada




If made of the same material and the only difference is the particle size, the spectra should not overlap and the spectral features should not change!

→ different composition?

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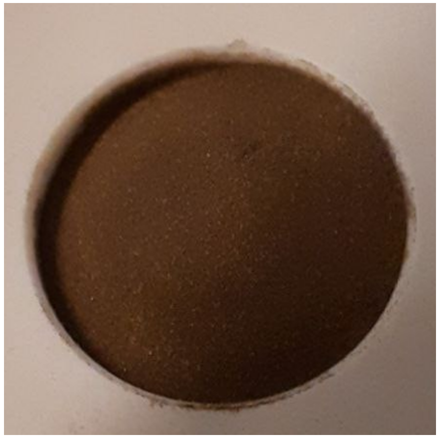
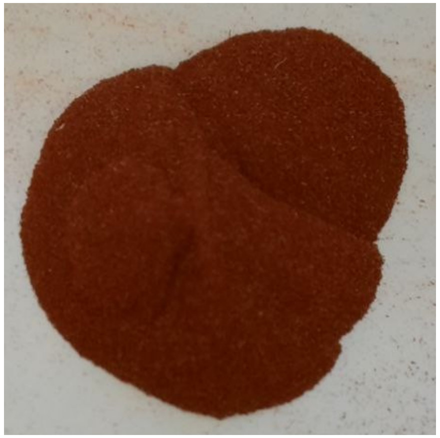
# Samples: final selection



63-100 µm samples are not homogeneous!
(larger quartz particles present)

→ only 20-40 µm samples can be used in the model as homogeneity is assumed

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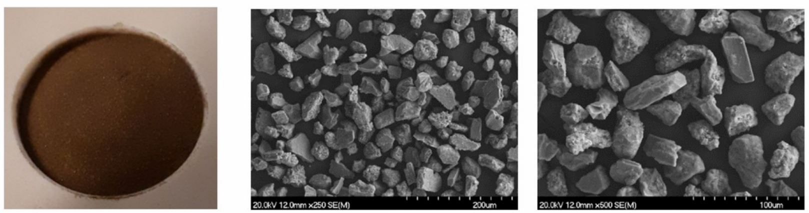
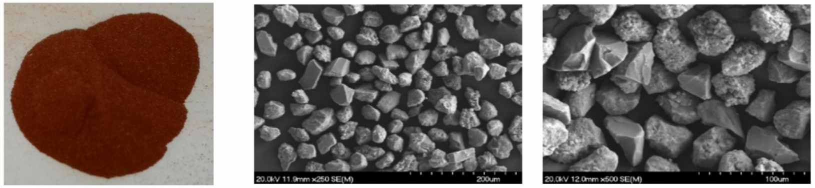
# Optical constants retrieval: samples

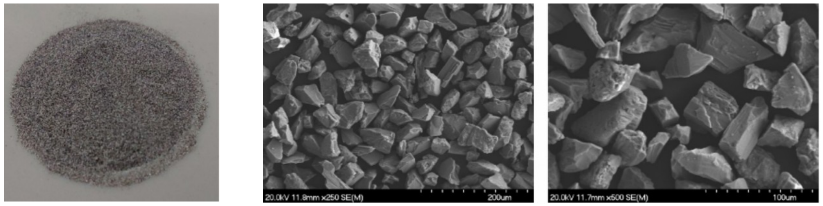
- 20-40 µm narrow size distributions in the geometric optics domain (r>>λ)
- MGS-1 added to the final selection



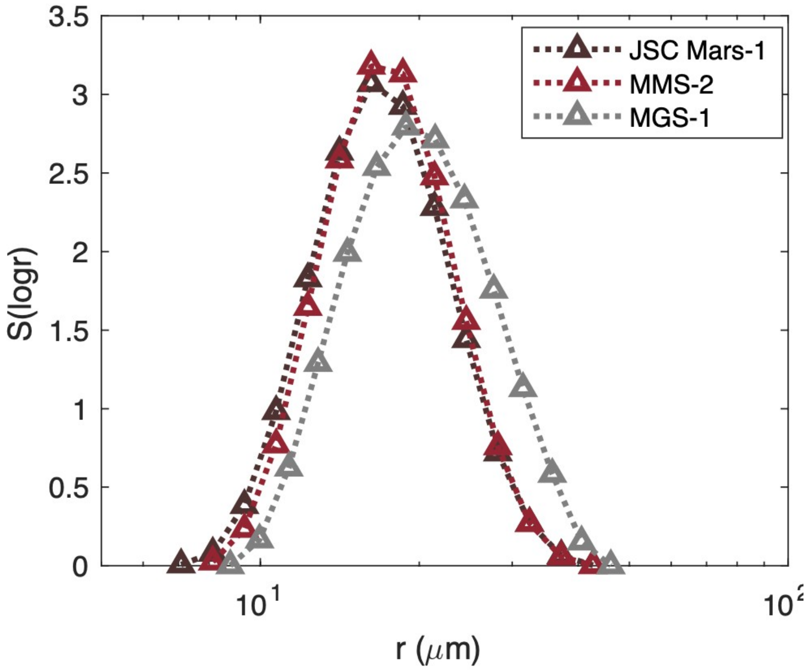
- JSC Mars-1 (Allen et al. 1997)



- Enhanced Mojave Mars Simulant (MMS-2, The Martian Garden)



- Mars Global Simulant (MGS-1, Cannon et al. 2019)

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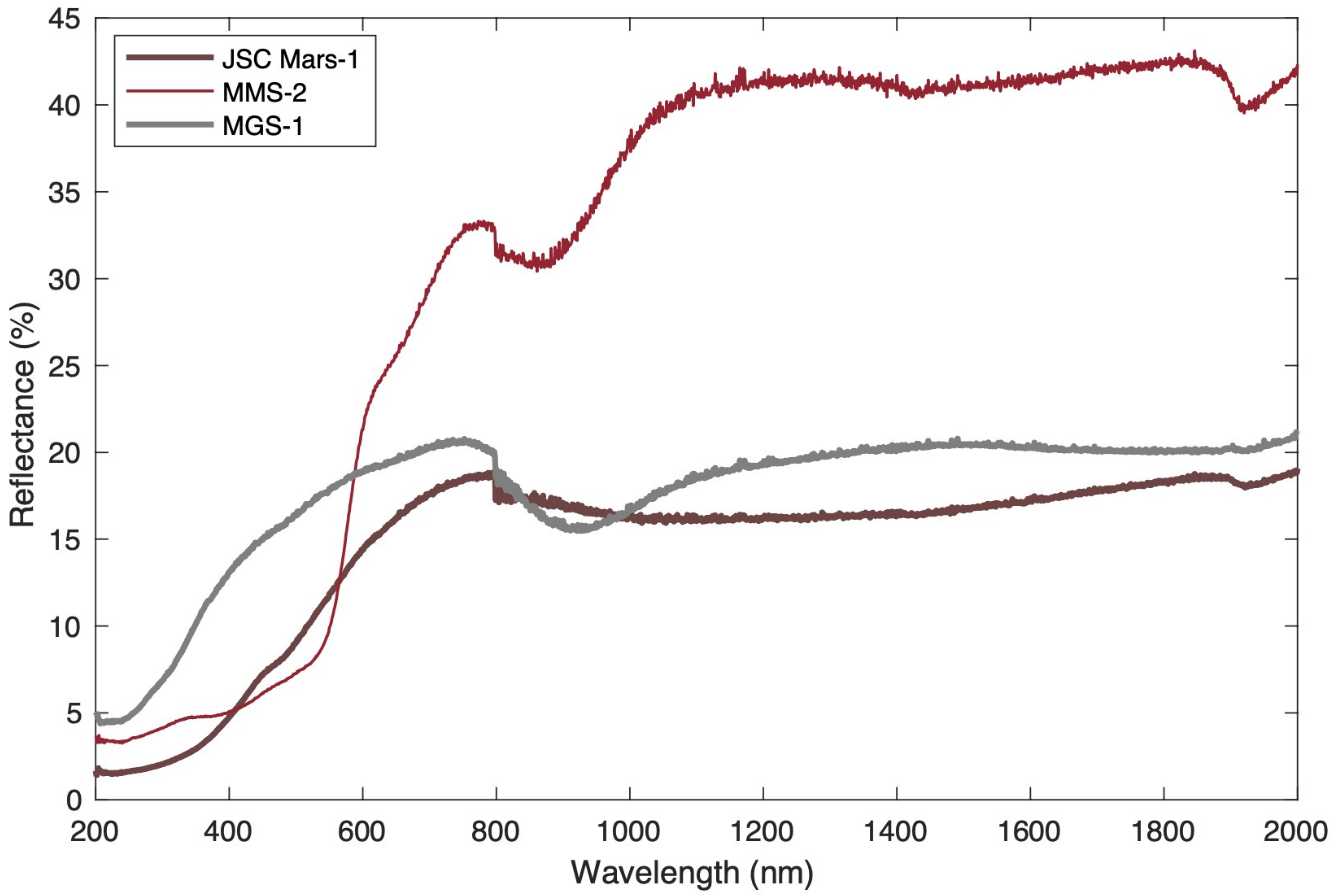
# Optical constants retrieval: Spectral measurements

- Diffuse reflectance spectra measured at Centro de Instrumentación Científica, University of Granada

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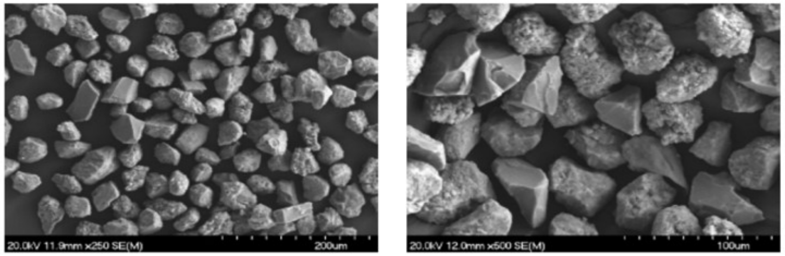
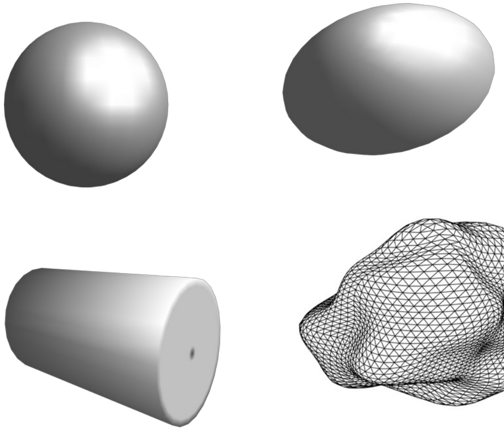
# Optical constants retrieval: particle shapes

- Light scattering computations are sensitive to the particle shapes




Field Emission Scanning Electronic Microscope (FESEM) image of the MMS-2 sample



?

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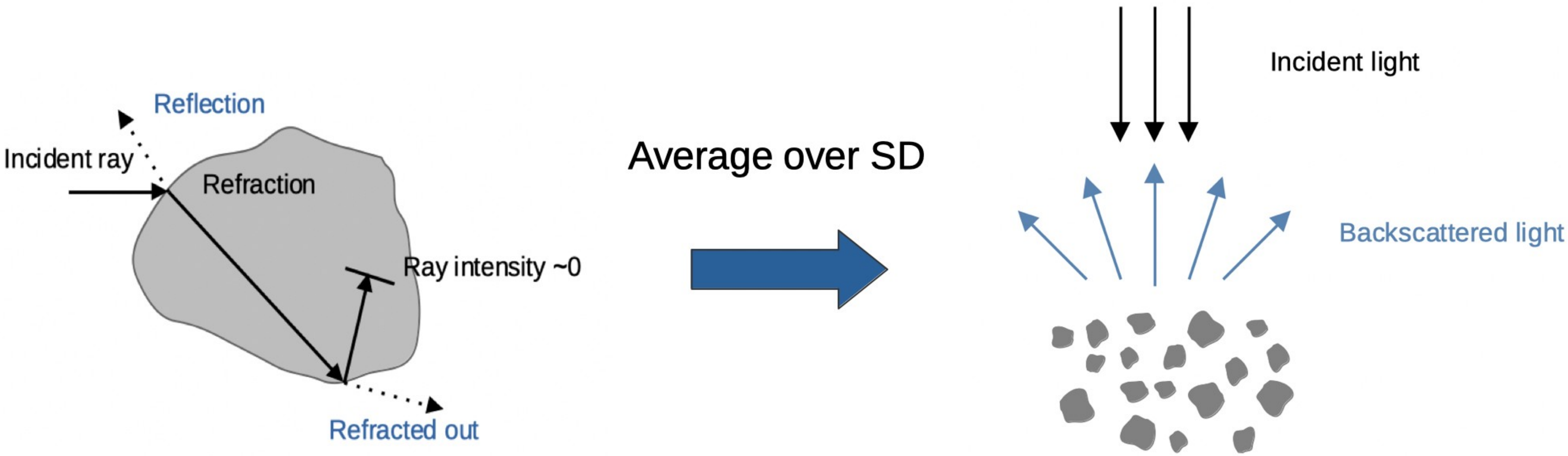
# Optical constants retrieval: methods

SIRIS4 (Muinonen et al. 2009, Lindqvist et al. 2018)

- simulates light scattering by Gaussian-random-sphere (GRS) particles larger than the wavelength of the incident light

RT-CB (Muinonen et al. 2004)

- multiple scattering




- n fixed to 1.5
- Approach: compute scattering properties for individual sizes (SIRIS4), average over the measured size distribution and use the averaged particles in RT-CB to simulate the surface → compare the retrieved reflectance with the measured spectral value → iterate

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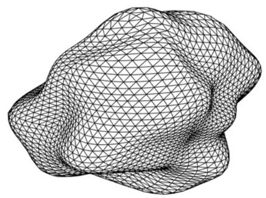
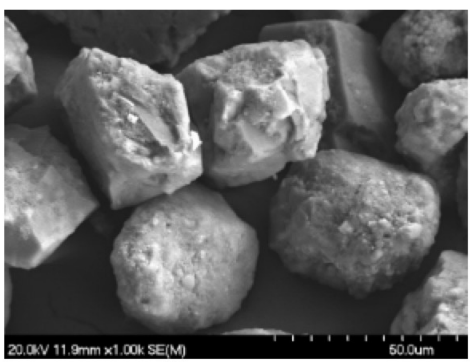
# Optical constants retrieval: first results

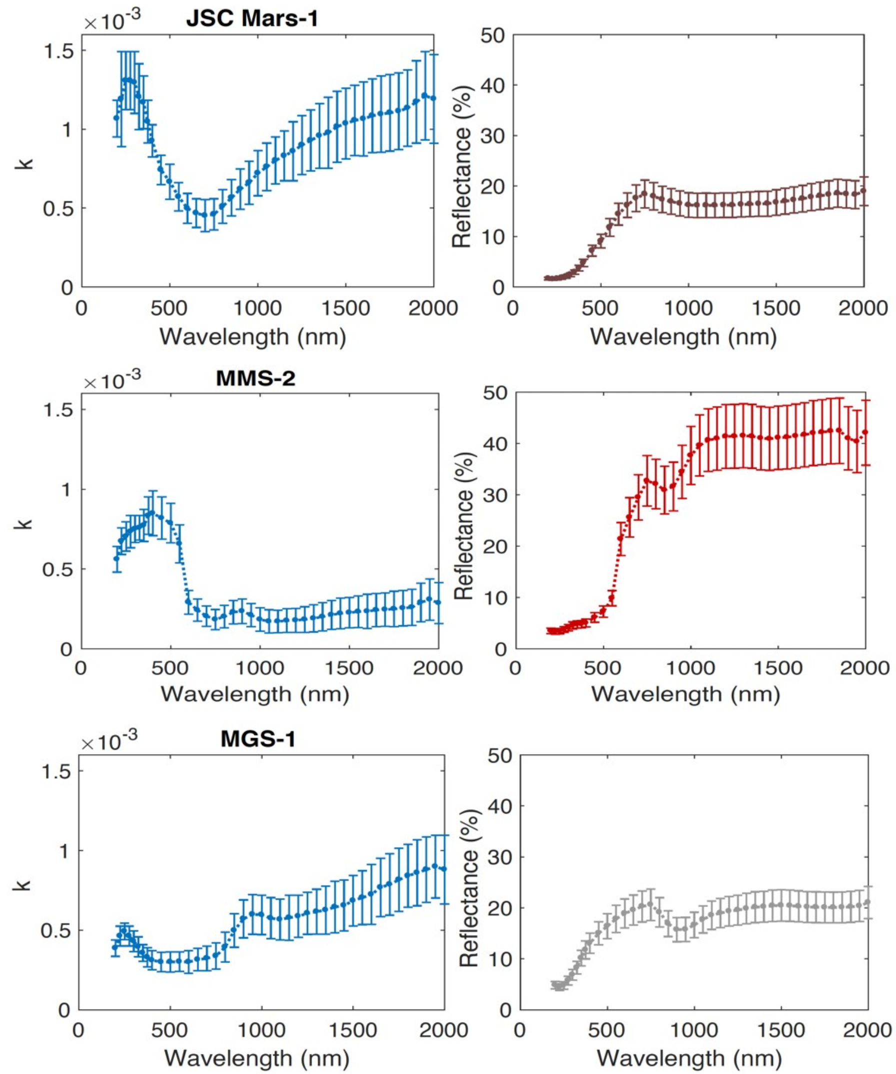


GRS1

- 15% maximum uncertainty assumed for the measured reflectance




MMS-2 FESEM image

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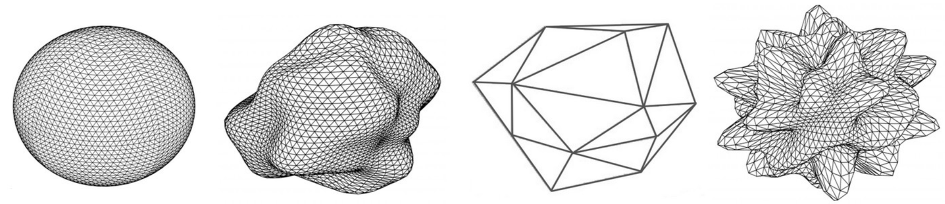
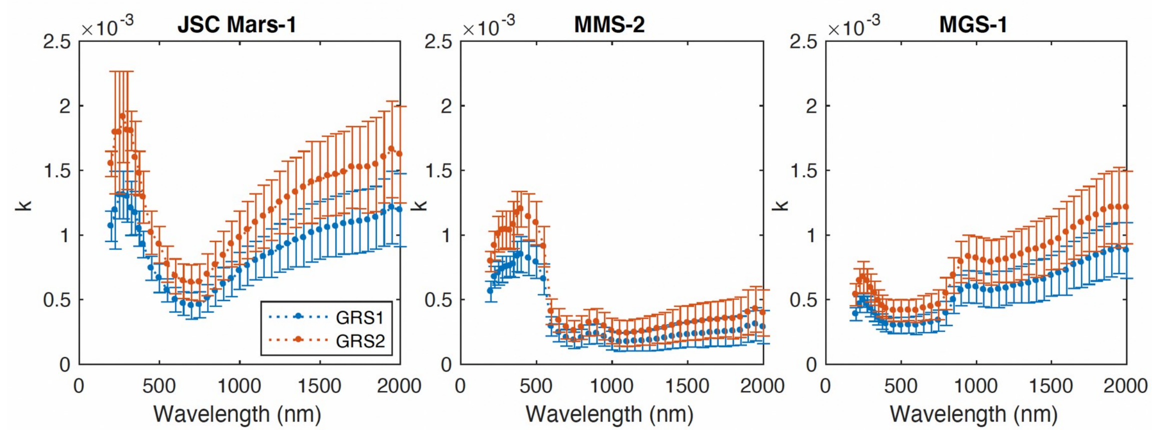
# Optical constants retrieval: shapes




| | λ (nm) | Sphere | GRS1 | **Polyhedra** | GRS2 |
|---|---|---|---|---|---|
| JSC Mars-1 | 400 | 0.000651 | 0.000926 | 0.000926 | 0.001292 |
| | 450 | 0.000514 | 0.000742 | 0.000758 | 0.001017 |
| | 500 | 0.000452 | 0.000666 | 0.000666 | 0.000926 |
| | 550 | 0.000384 | 0.000571 | 0.000578 | 0.000773 |
| | 600 | 0.000330 | 0.000498 | 0.000510 | 0.000681 |
| | 650 | 0.000315 | 0.000468 | 0.000481 | 0.000643 |
| MMS-2 | 400 | 0.000620 | 0.000849 | 0.000869 | 0.001200 |
| | 450 | 0.000575 | 0.000819 | 0.000842 | 0.001139 |
| | 500 | 0.000544 | 0.000788 | 0.000815 | 0.001093 |
| | 550 | 0.000452 | 0.000658 | 0.000669 | 0.000910 |
| | 600 | 0.000193 | 0.000292 | 0.000304 | 0.000407 |
| | 650 | 0.000159 | 0.000243 | 0.000250 | 0.000338 |
| MGS-1 | 400 | 0.000210 | 0.000311 | 0.000320 | 0.000430 |
| | 450 | 0.000201 | 0.000300 | 0.000311 | 0.000414 |
| | 500 | 0.000201 | 0.000300 | 0.000306 | 0.000416 |
| | 550 | 0.000201 | 0.000302 | 0.000307 | 0.000416 |
| | 600 | 0.000199 | 0.000300 | 0.000309 | 0.000414 |
| | 650 | 0.000208 | 0.000315 | 0.000320 | 0.000433 |




- The derived *k* **increases** when the particle irregularity **increases**

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# Optical constants retrieval: n

| | $\lambda$ (nm) | $n = 1.4$ | $n = 1.5$ | $n = 1.6$ |
|---|---|---|---|---|
| JSC Mars-1 | 200 | 0.000946 | 0.001067 | 0.001138 |
| | 300 | 0.001211 | 0.001296 | 0.001467 |
| | 400 | 0.000864 | 0.000926 | 0.000956 |
| | 450 | 0.000712 | 0.000742 | 0.000742 |
| | 500 | 0.000651 | 0.000666 | 0.000666 |
| | 550 | 0.000552 | 0.000571 | 0.000559 |
| | 600 | 0.000483 | 0.000498 | 0.000483 |
| | 650 | 0.000460 | 0.000468 | 0.000460 |
| | 1000 | 0.000709 | 0.000721 | 0.000709 |
| | 1250 | 0.000904 | 0.000899 | 0.000880 |
| | 1500 | 0.001028 | 0.001036 | 0.001017 |
| | 1750 | 0.001096 | 0.001104 | 0.001085 |
| | 2000 | 0.001183 | 0.001192 | 0.001163 |
| MMS-2 | 200 | 0.000523 | 0.000561 | 0.000583 |
| | 300 | 0.000719 | 0.000751 | 0.000783 |
| | 400 | 0.000819 | 0.000849 | 0.000864 |
| | 450 | 0.000803 | 0.000819 | 0.000834 |
| | 500 | 0.000773 | 0.000788 | 0.000788 |
| | 550 | 0.000643 | 0.000658 | 0.000658 |
| | 600 | 0.000292 | 0.000292 | 0.000284 |
| | 650 | 0.000245 | 0.000243 | 0.000239 |
| | 1000 | 0.000184 | 0.000184 | 0.000178 |
| | 1250 | 0.000189 | 0.000184 | 0.000182 |
| | 1500 | 0.000230 | 0.000227 | 0.000221 |
| | 1750 | 0.000255 | 0.000250 | 0.000238 |
| | 2000 | 0.000289 | 0.000287 | 0.000273 |
| MGS-1 | 200 | 0.000372 | 0.000387 | 0.000402 |
| | 300 | 0.000420 | 0.000431 | 0.000442 |
| | 400 | 0.000308 | 0.000311 | 0.000311 |
| | 450 | 0.000300 | 0.000300 | 0.000300 |
| | 500 | 0.000300 | 0.000300 | 0.000294 |
| | 550 | 0.000296 | 0.000302 | 0.000292 |
| | 600 | 0.000300 | 0.000300 | 0.000296 |
| | 650 | 0.000311 | 0.000315 | 0.000308 |
| | 1000 | 0.000590 | 0.000596 | 0.000587 |
| | 1250 | 0.000597 | 0.000606 | 0.000587 |
| | 1500 | 0.000675 | 0.000685 | 0.000665 |
| | 1750 | 0.000811 | 0.000816 | 0.000802 |
| | 2000 | 0.000860 | 0.000880 | 0.000841 |

- Is it OK to assume $n$ = 1.5 over the entire wavelength range?
- The derived $k$ is not sensitive to the changes in $n$ when the retrieval is carried out using the measured reflectance spectrum

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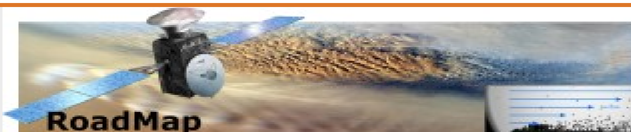

# Optical constants retrieval: validation

- How well do the analogues represent the Martian surface?
- The observed NOMAD UVIS spectrum (Willame et al. 2022):  a relatively high visible albedo region with a limited impact from the atmosphere;  no ice clouds, the amount of dust was low, and the solar zenith angle was small
- Bidirectional reflectance computations carried out using the derived refractive indices, SIRIS4, and Radiative Transfer and Coherent Backscattering (RT-CB) code (Muinonen et al. 2004)

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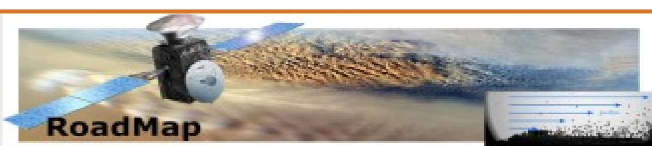
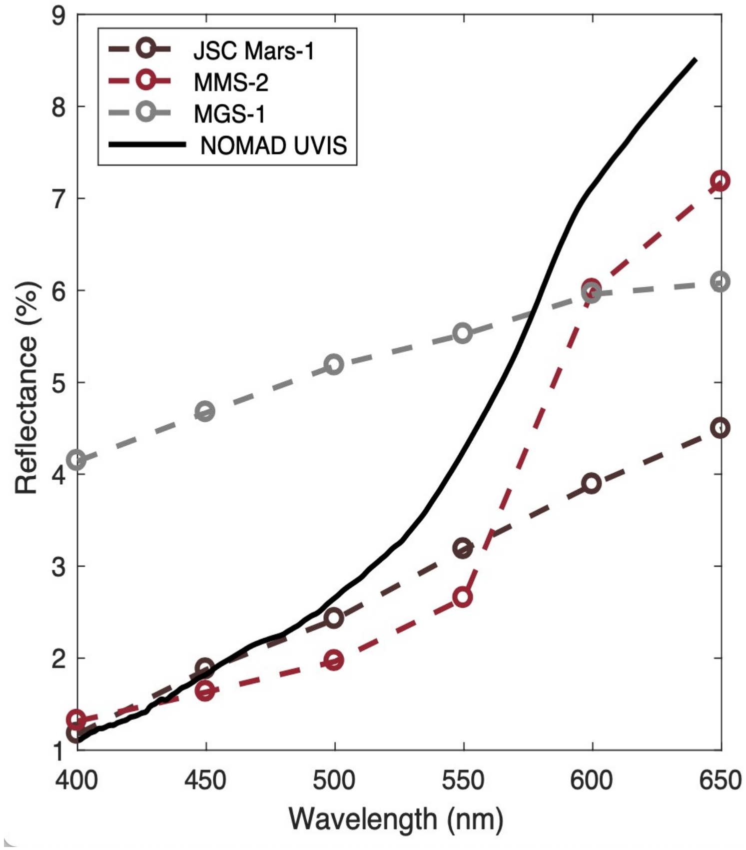


# Optical constants retrieval: validation




SD 20-40 μm

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# Optical constants retrieval: validation

- Previous studies: particle sizes < 100 µm, bright region particle SD can be in the range of 2 – 40 µm (Ruff & Christensen 2002, Christensen 1986)
- To better simulate the surface, we created a broad normal size distribution in the range of 2-40 µm and repeated the bidirectional reflectance computations for the MMS-2 analogue
- Compared with computations that were performed by using the optical constants in the literature (Wolff et al. 2009)

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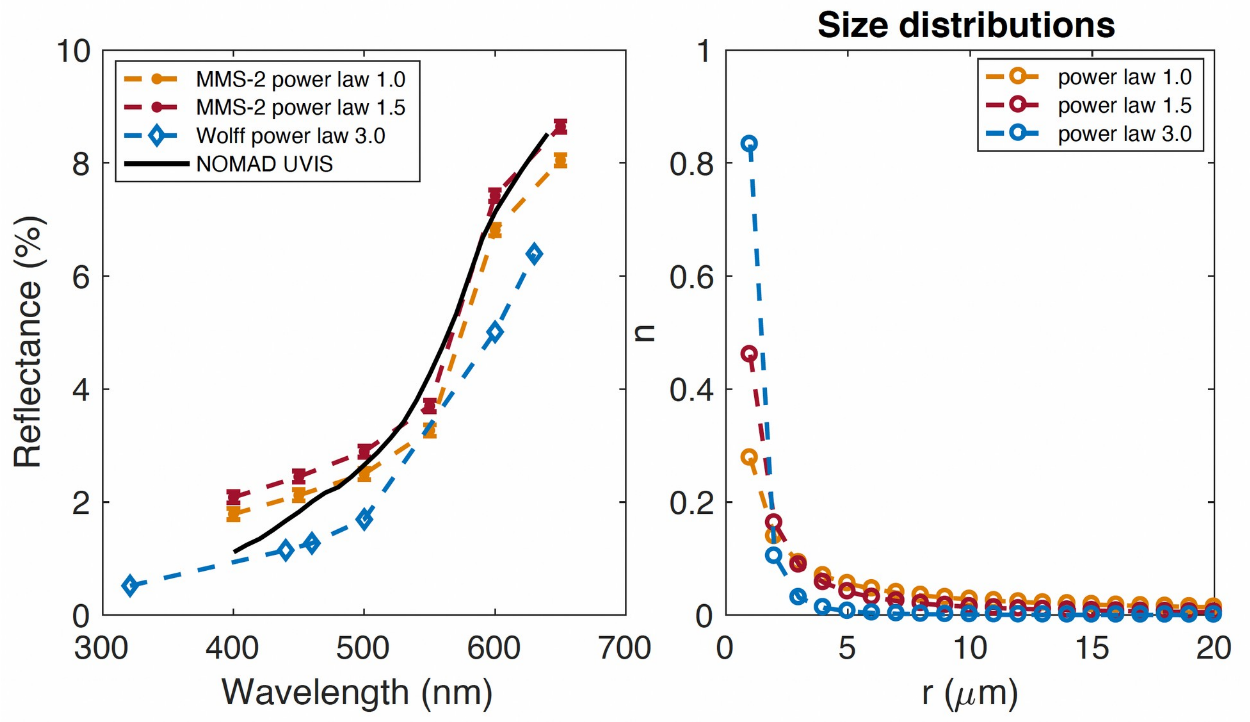
# Optical constants retrieval: validation




- Modelled slope in the UV not as steep as for the observed spectrum
- Differences between the retrieved k and the values in the literature could be explained by:

  - different particle shapes

  - different composition of the surface regolith compared to the lifted atmospheric dust (compositional separation??)

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# Compositional separation?

**MMS-2 20-40 µm**

- The composition changes slightly when separating the particles by size. According to XRD, the 20-40 µm fraction shows quartz as the main phase, which explains the more whitish colour of the powder. For this reason, this fraction was again prepared from the previously milled MMS-2 powder.
- To what extent could the compositional separation operate on Mars?

Published in Martikainen et al. 2023, ApJS (in press)

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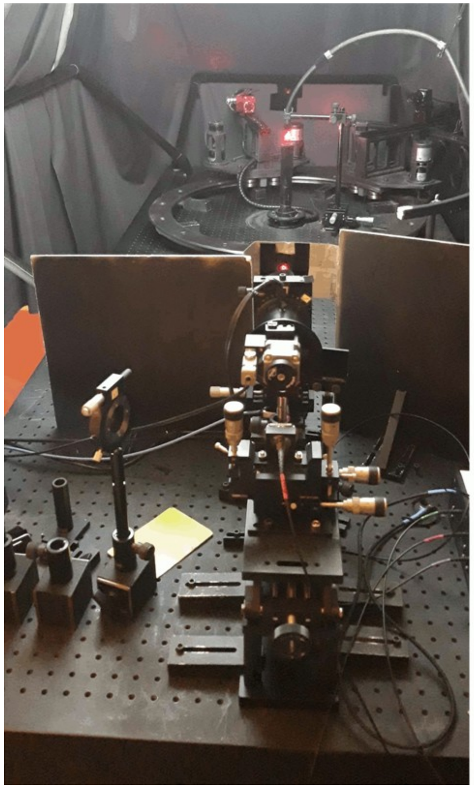
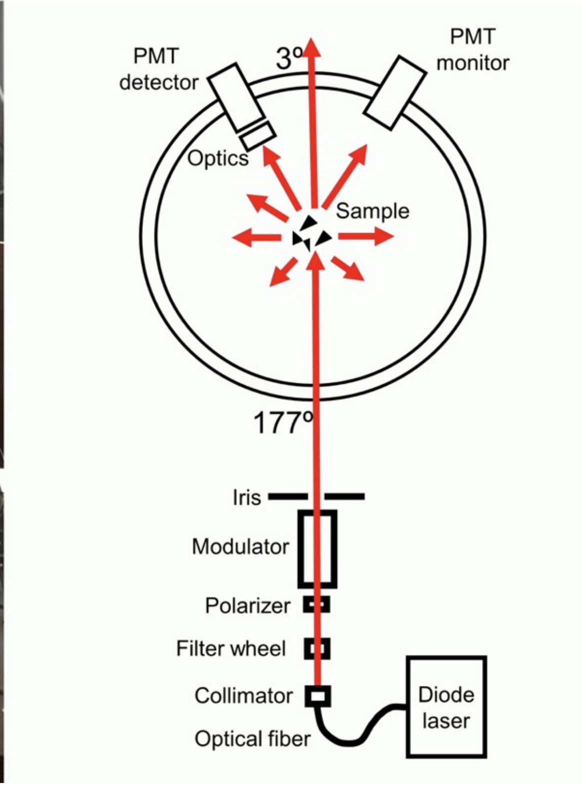
# Scattering properties: measurements

- COsmic DUst LABoratory (CODULAB, Muñoz et al. 2012 )
  → measure the scattering matrix elements F11, F12, F22, F33, F34, and F44 of the Martian dust analogues at 488nm and 640nm

- Retrieval of the **scattering properties** by using the known particle size distributions, measured scattering matrix elements, derived complex refractive indices, and a scattering database



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# Scattering properties: approach

- Two approaches:

  **1.** Compute the scattering properties from the scratch using advanced numerical methods
  - Problem: various particle size distributions and materials, computationally heavy. Changing parameters results in new computations.

  **2**. Use a scattering database to retrieve the scattering properties
  - Pre-calculated scattering properties over a wide range of particle sizes, refractive indices, and wavelengths

- How to select the "ideal" particle shape?
  - Try to reproduce the laboratory measurements by using databases that utilize different particle shapes
  → use the database that produces the best fit

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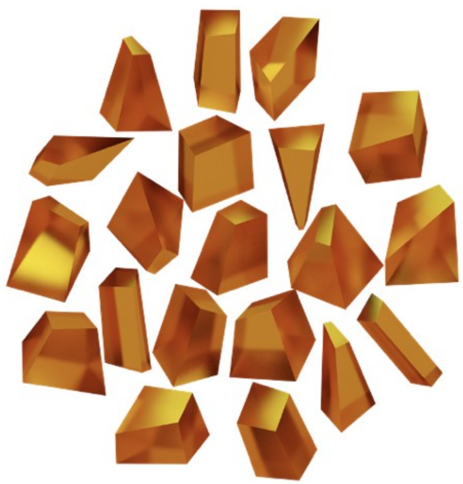
# Scattering properties: scattering databases



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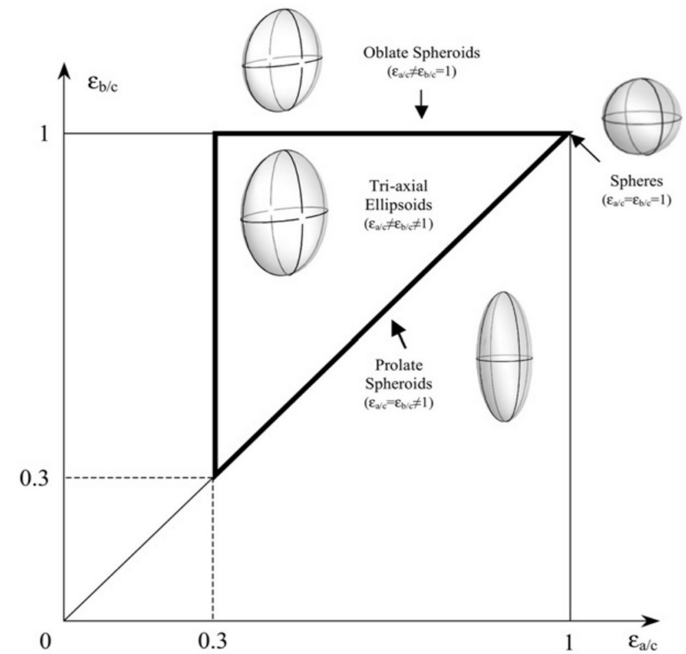


TAMUdust2020, Saito et al. 2021

Tri-axial ellipsoids, Meng et al. 2010

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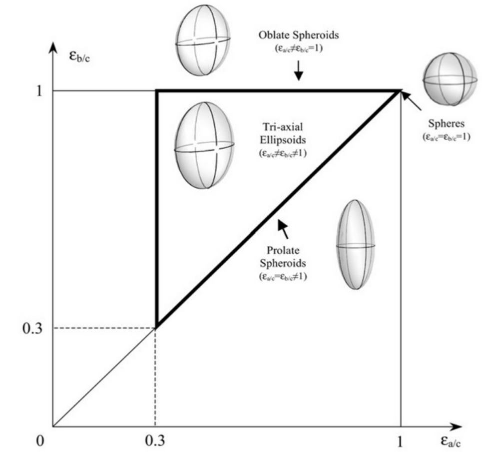
# Scattering properties: tri-axial ellipsoids




- Download: https://zenodo.org/record/4959767#.YnjcCC0RrRX
- Tri-axial ellipsoid database by Meng et al. 2010

  - Pre-calculated data:
    - 42 shapes
    - Axis ratios ranging from 1 to 3.3
    - 69 refractive indices: $m_{re} \in [1.1, 2.1]$, $m_{im} \in [0.0005i, 0.5i]$
    - 471 entries for size parameters, **x**, ranging from 0.025 to 1000

- 34 shapes selected: contain 1 sphere, 6 prolate and 6 oblate spheroids, ellipsoids
  - Nearly spherical shapes were omitted (Merikallio et al. 2013)
  - Equiprobable shape distribution

average

$$P(\theta) = \frac{\sum_i \eta_i \sum_r n_r C_{\text{sca}}(r,i) P(\theta,r,i)}{\sum_i \eta_i \sum_r n_r C_{\text{sca}}(r,i),}$$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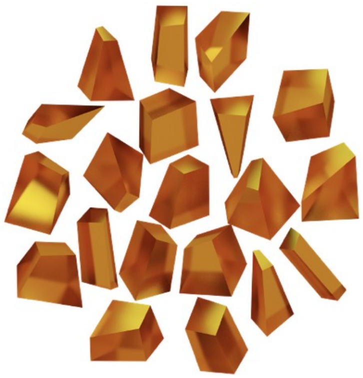
# Scattering properties: hexahedra

- Download: https://sites.google.com/site/masanorisaitophd/data-and-resources/tamudust2020
- Ensemble of 20 hexahedral particles
- SW (shortwave) and LW (longwave) domains
  - SW: $m_{re}$ = 1.37 – 1.7, $m_{im}$ = 0.0001 – 0.1, **x** ranges from Rayleigh to 11800
  - LW: $m_{re}$ = 0.4 – 3.2, $m_{im}$= 0.001-4.0, **x** ranges from Rayleigh to 1450



- Sphericity parameter defines the mixing rate of different irregular shapes within the ensemble (0.695 – 0.785)
  - Small value → higher aspect ratio
  - 0.695 for dust particles

average

$$\langle \mathbf{P}(\theta) \rangle = \frac{\int_{D_{\min}}^{D_{\max}} n(D) A(D,\Psi) Q_{sca}(D,m_r,m_i,\Psi) \mathbf{P}(\theta,D,m_r,m_i,\Psi)\, dD}{\int_{D_{\min}}^{D_{\max}} n(D) A(D,\Psi) Q_{sca}(D,m_r,m_i,\Psi)\, dD}.$$

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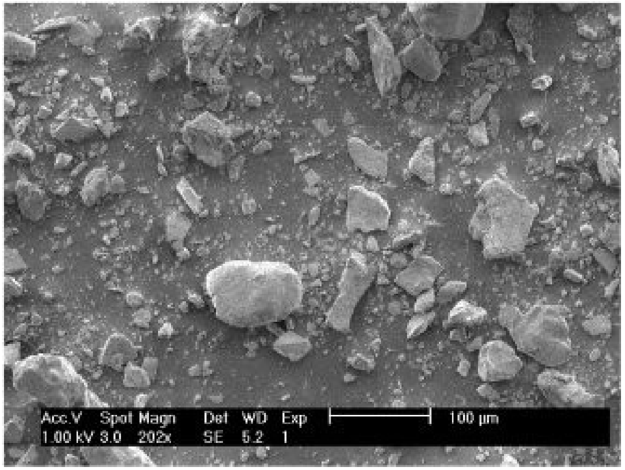
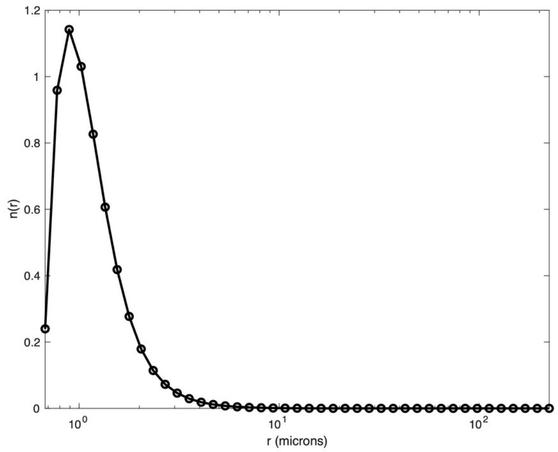
# Scattering properties: palagonite test

- Scattering matrix measurements of palagonite at 632.8nm
- Testing with spheres, tri-axial ellipsoids, and hexahedra shapes
- Complex refractive index m fixed to 1.6+i0.0005 according to the best-fit solution carried out by Merikallio et al. 2013

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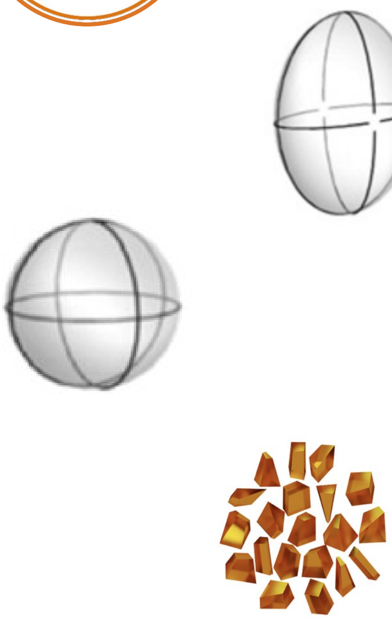
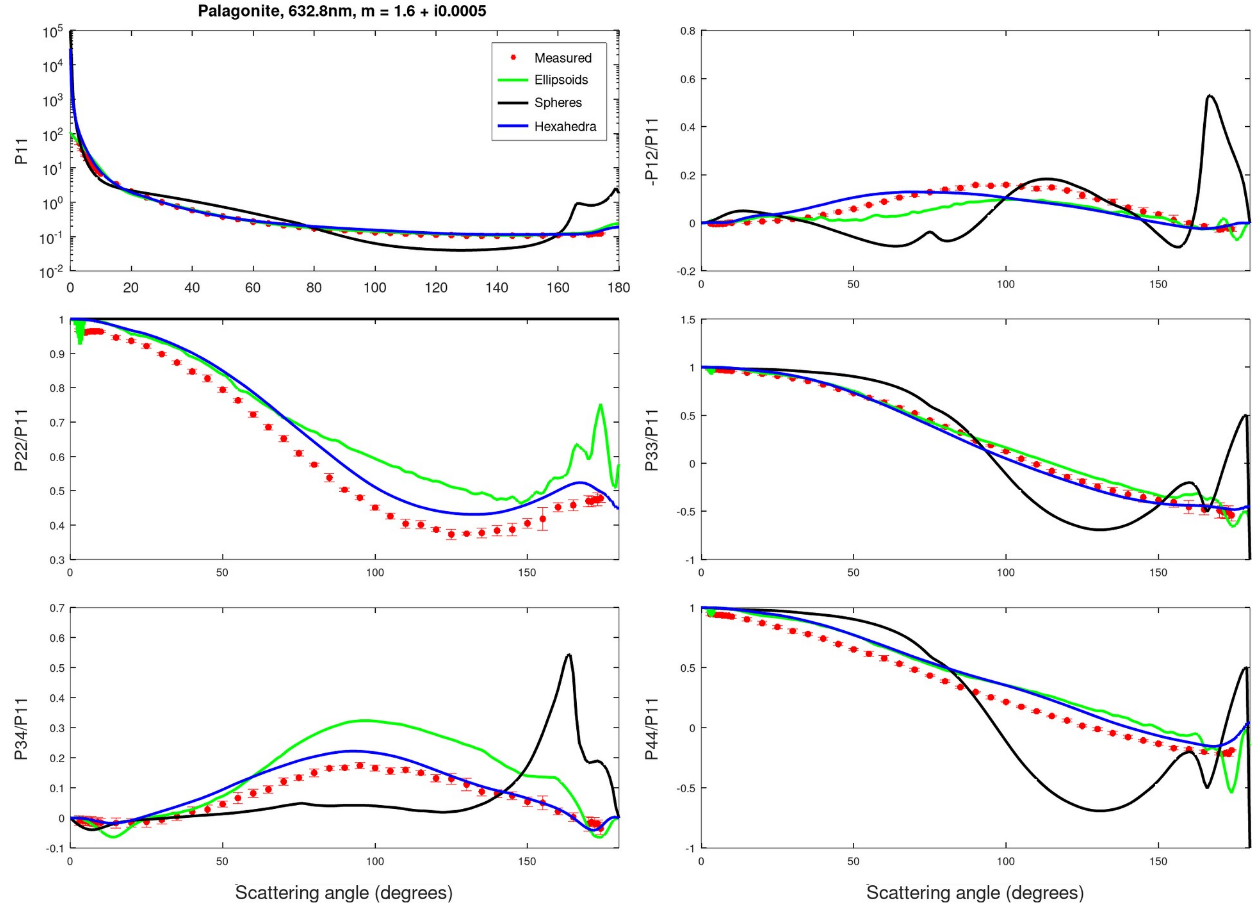
# Scattering properties: palagonite test






The hexahedra database produces best fits
→ selected to be used for the scattering properties retrieval of Martian dust

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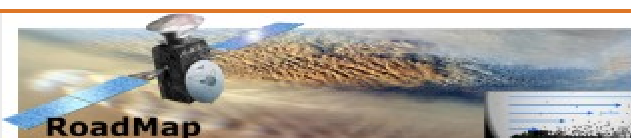
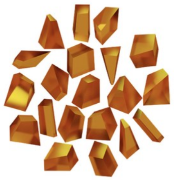
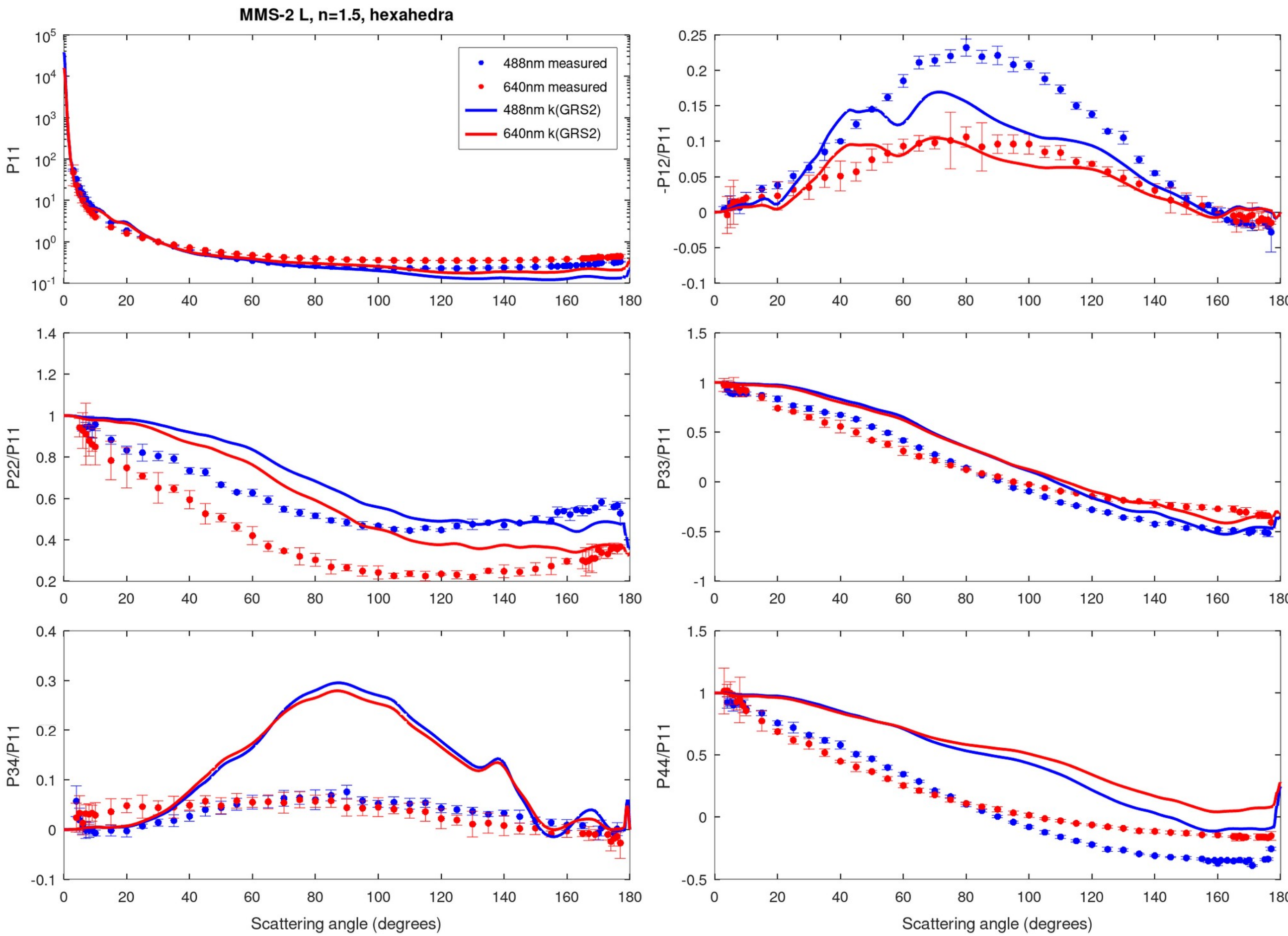


# Scattering properties: MMS-2 SD L

- Single-scattering properties modelled using the hexahedra database + *k*(GRS2) + measured SD



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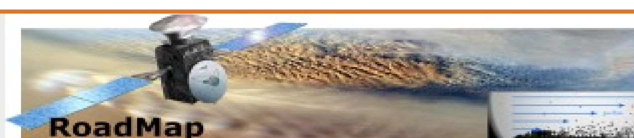
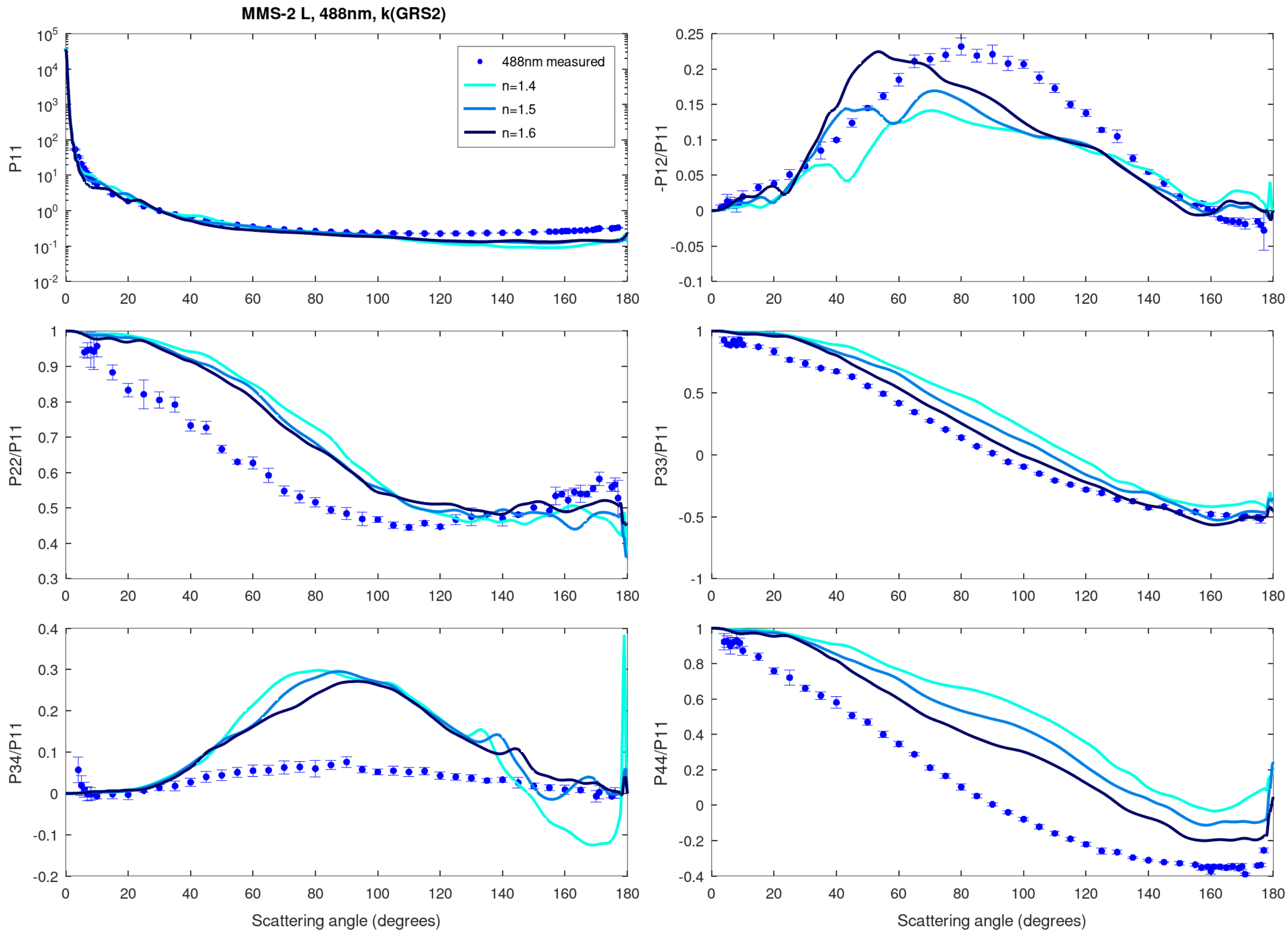


# Scattering properties: MMS-2 SD L

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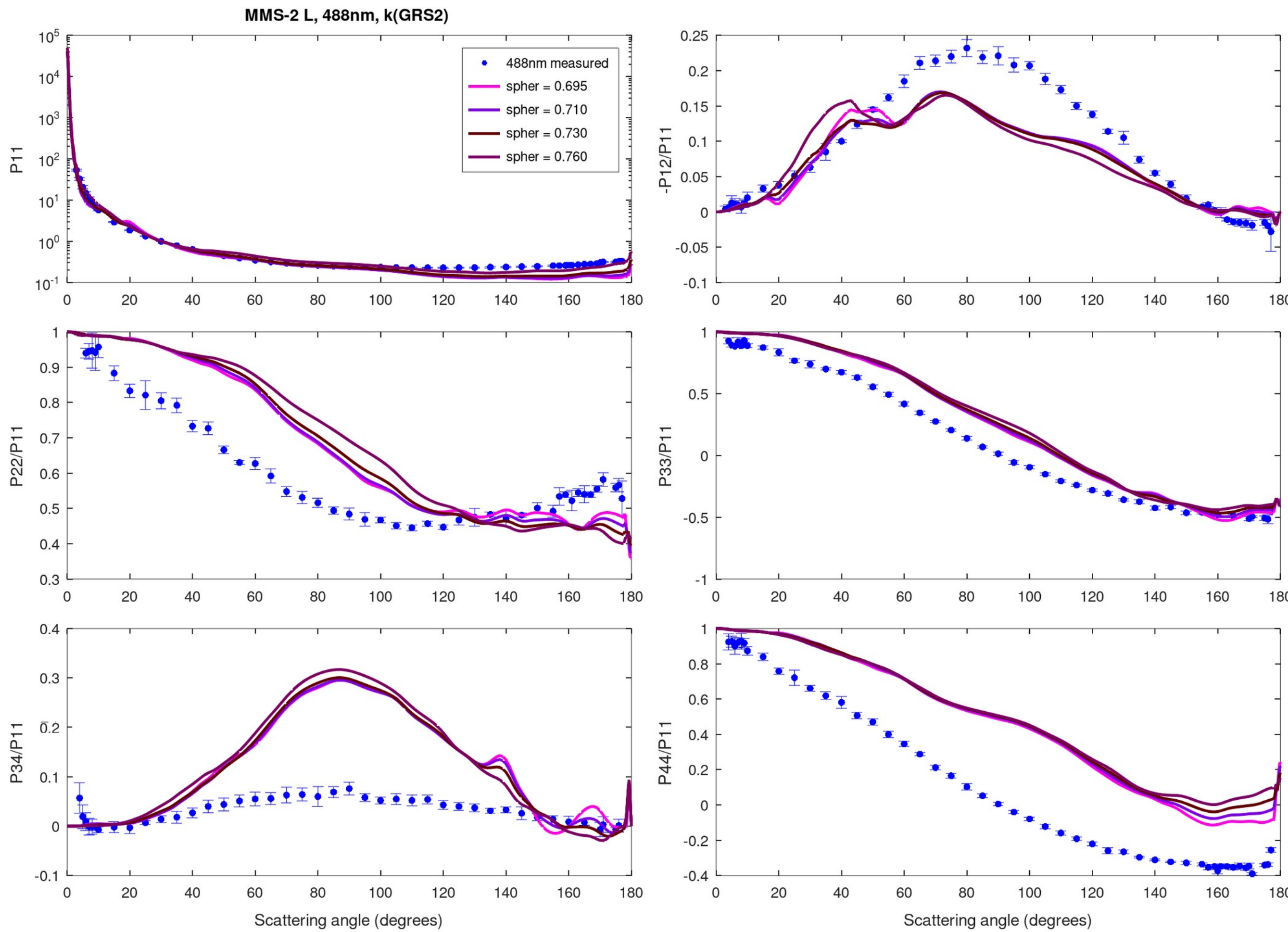
# Scattering properties: MMS-2 SD L

- Sphericity

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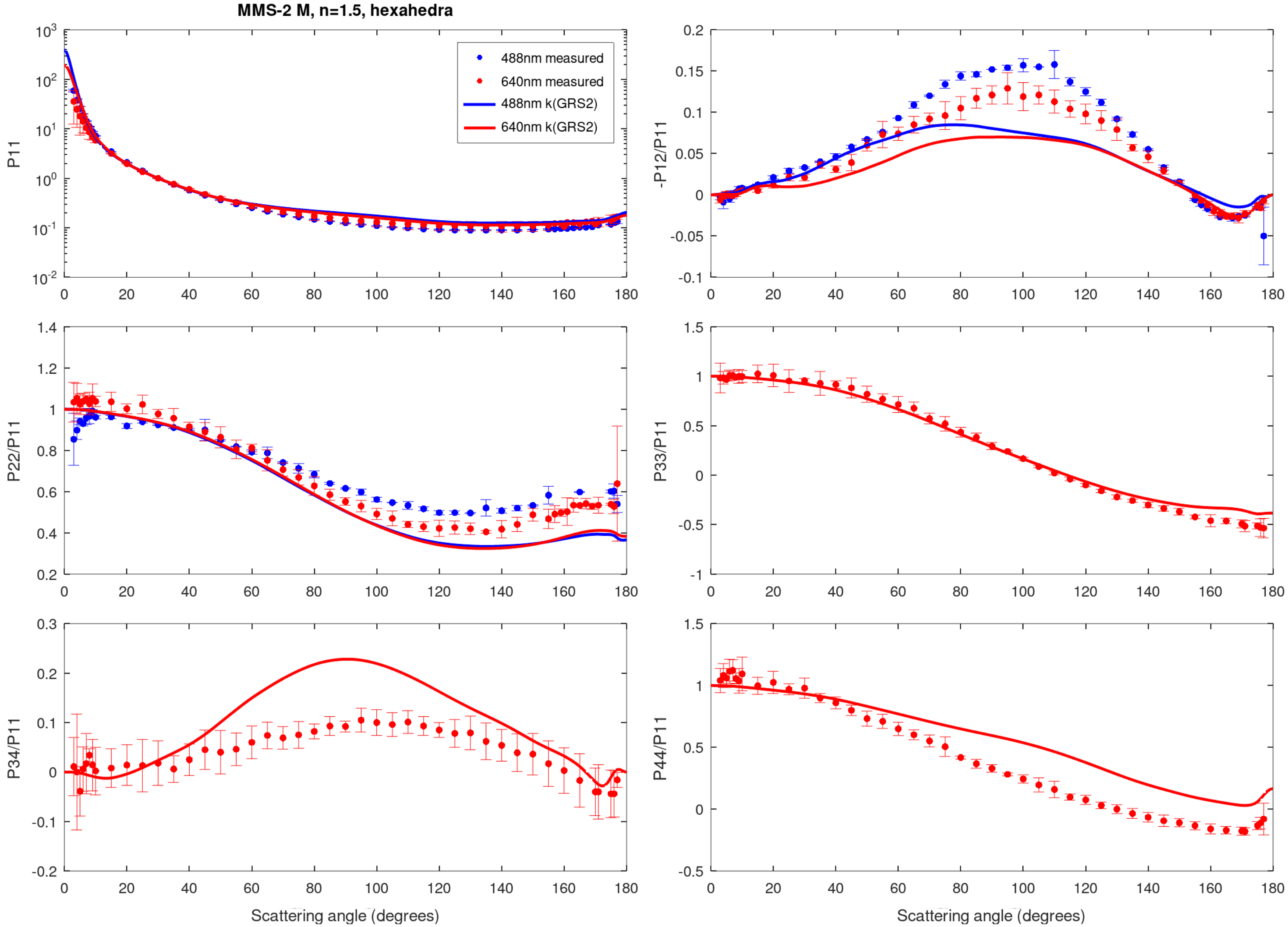
# Scattering properties: MMS-2 SD M

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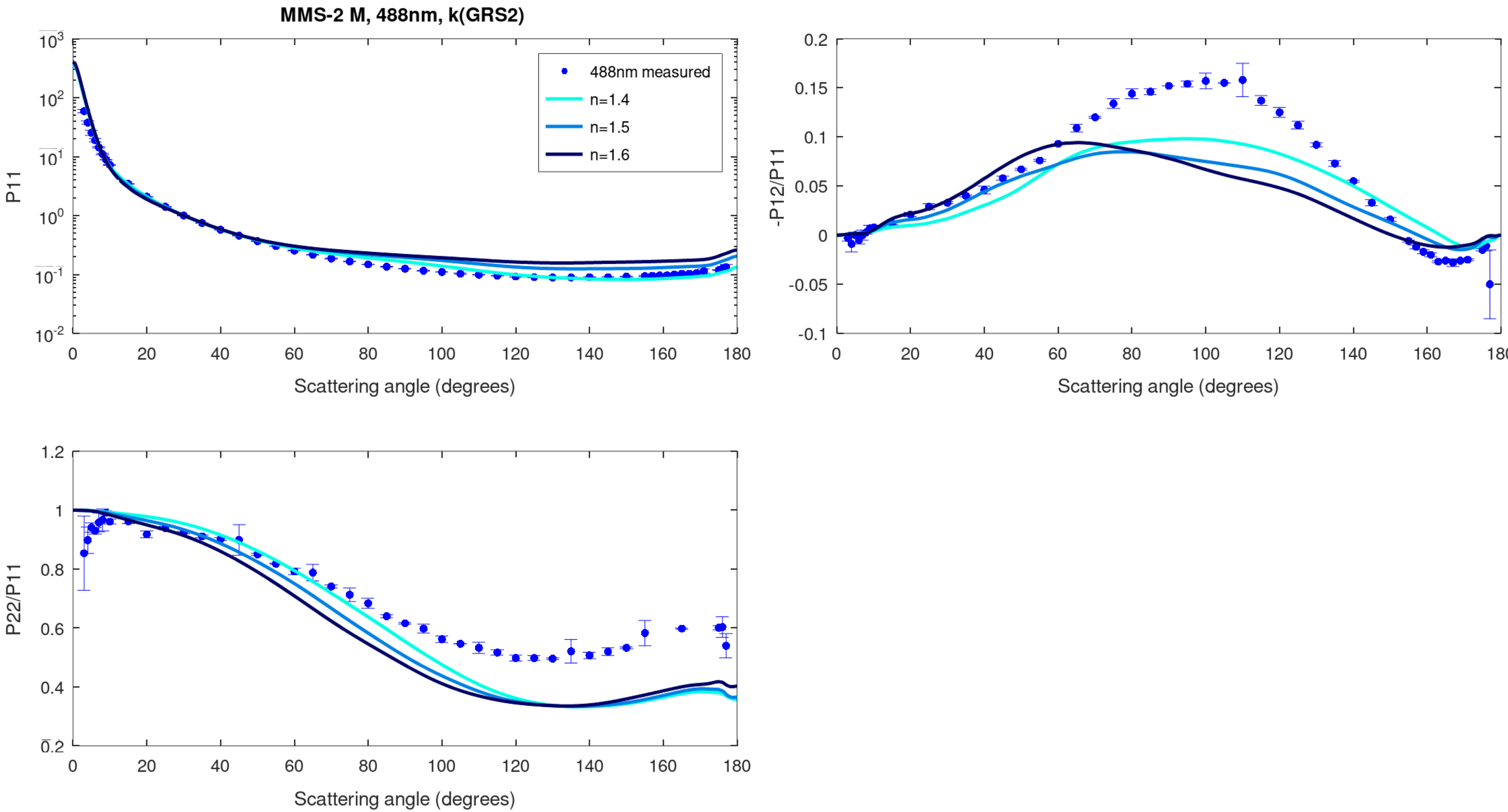
# Scattering properties: MMS-2 SD M

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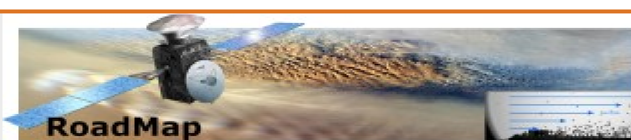

# Summary

- We used an advanced light scattering model together with laboratory measurements to retrieve optical constants for three martian dust analogues: JSC Mars-1, MMS-2, and MGS-1

  - Sensitivity tests showed that the retrieved values are sensitive to the particle shape

- The selected particle shape should reproduce well the measured reflectance spectrum and the scattering matrix

  - Spheres, tri-axial ellipsoids, and hexahedra particles were tested on palagonite → the hexahedra particles produced the best fits to the measurements

- We are currently working on retrieving the scattering properties of martian dust analogues from their measured scattering matrices by using the derived optical constants, measured particle size distributions, and the hexahedra database

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