



# EUROPLANET 2020-RI - VESPA WP

## European Data Bases Infrastructure of Solid Spectroscopy



# **SSHAD**

*Solid Spectroscopy Hosting Architecture of Databases & Expertise*

<https://www.sshade.eu>

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Damien Albert, Lydie Bonal and the SSHAD Consortium Partners



# The SSHADe database infrastructure

for Astrophysics, Planetary sciences and Geosciences

A set of databases of **spectra of solids**



in the **electromagnetic spectrum**

**From a Consortium of laboratories**

hosted by **OSUG Data Center/UGA** in Grenoble, France

# SSHADE European Consortium of Data Providers

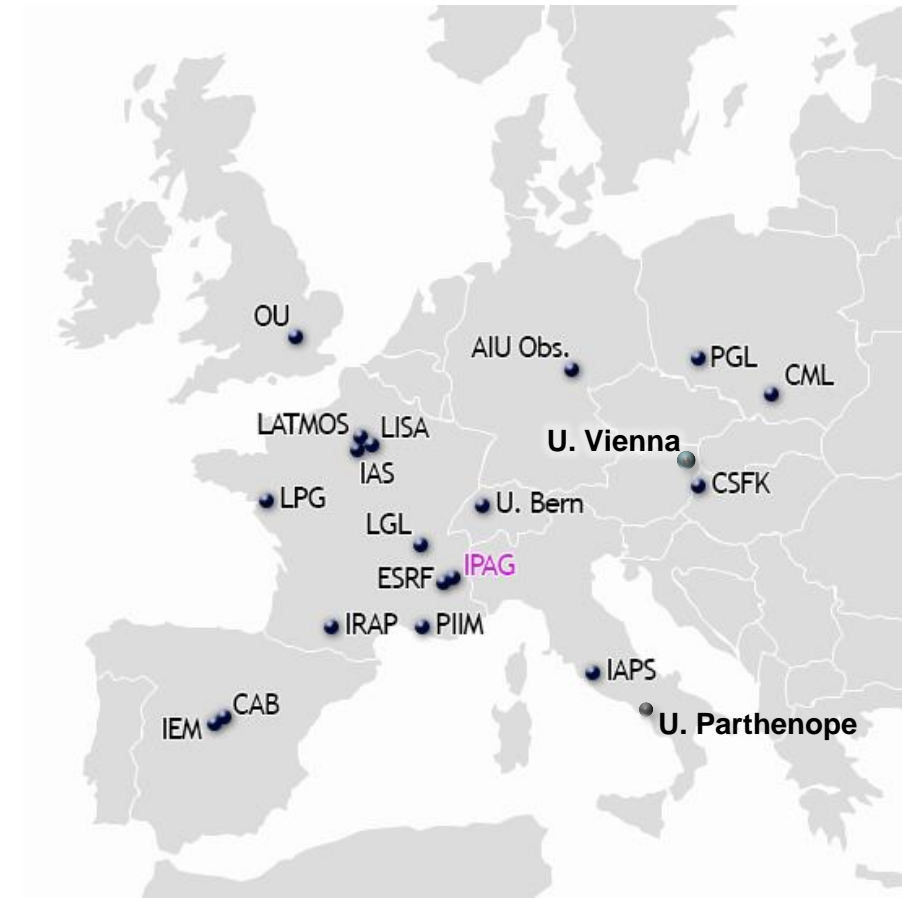
Data from **23** solid spectroscopy experimental groups  
in **8** European countries (F, PL, D, GB, CH, E, I, HU) +India +Taiwan  
~**75** researchers

**Each with particular expertise on:**

- some wavelength ranges
- type of materials and physico-chemical conditions
- specific techniques
- type of data and products, ...

**13 active databases + 4 starting + 2 coming**

SSHADE Wiki : <https://wiki.sshade.eu>



# Main aim of *SSHADE*

- **Provide to the planetary and astrophysics community**
  - **Spectral and spectro-photometric data**
    - over all the electromagnetic spectrum
    - on all types of solid materials (but also liquid)
    - from synthetic, terrestrial or extraterrestrial samples
  - **With well documented information**
    - on the spectra, samples, experiments ...
  - **From a set of cutting edge experimental laboratories**
    - From Europe, Asia, ...
- **For the analysis, modeling and interpretation of spectroscopic observations of planetary surfaces, aerosols & grains, + inter- & circumstellar grains, exoplanets...**

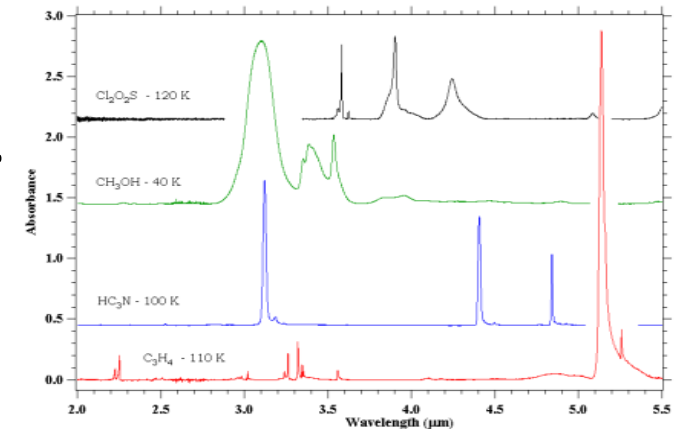
# Which types of materials and samples in *SSHADE* ?

- **Materials**

- **Ices** (low/high T-P, mixtures, ...), molecular solids, snow...
- **Minerals**, rocks
- **Organic solids**, polymers, **Carbonaceous materials**, ...
- **Inorganic solids**, Metals, ...
- also some **liquids**

- **Samples**

- **Synthesized** in the laboratory
- **Natural terrestrial analogues** collected or measured in the field
- **Cosmomaterials collected on Earth**: (micro-)meteorites, *IDPs*, ...
- **Extra-terrestrial samples** collected on planetary bodies: lunar soils...



# Which types of spectra in SSHADE ?

- **Spectral ranges:**

- Designed from g-rays to radio wavelengths
- Now mostly **from near-UV to sub-mm (0.3 $\mu\text{m}$  - 1mm)**, plus **X-rays**.

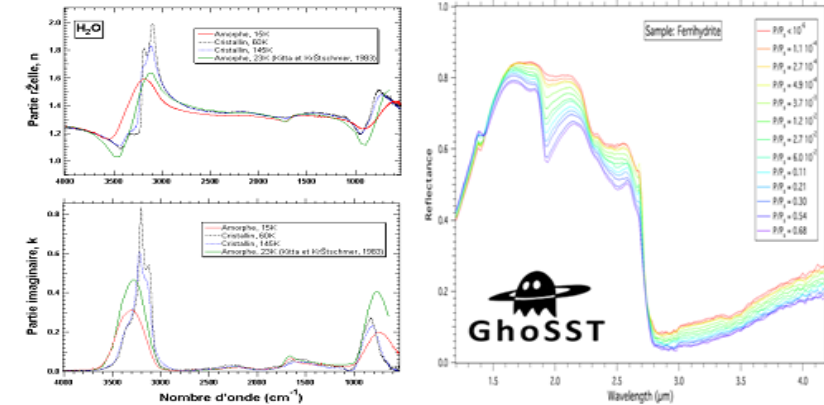
- **Types of data:**

- **Spectra**

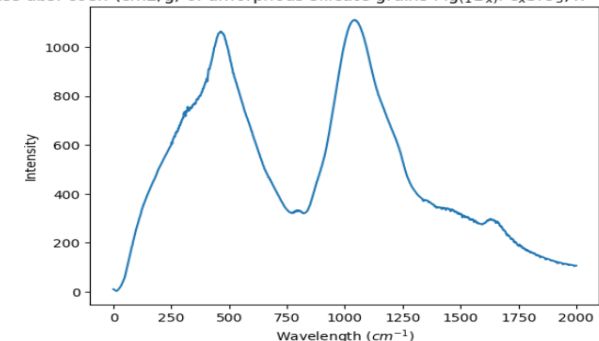
- **Transmission** spectra, absorption coefficients, **optical constants** ...
- **Reflectance** spectra of surfaces, spectro-photometric functions, ...
- **Raman** spectra & micro-spectroscopy, *Fluorescence*, ...
- **XANES** spectra

- **Bandlist** (under development ... → mid-2019)

- *position, width, intensity, vibration modes* ... **for molecular solids**



Mass abs. coef. (cm<sup>2</sup>/g) of amorphous silicate grains Mg<sub>(1-x)</sub>Fe<sub>x</sub>SiO<sub>3</sub>, x=0.3



# Examples of SSHADE data

**GhoSST**  
(IPAG – F)

MIR-FIR  
optical constants  
of ices

*H<sub>2</sub>O ice crystalline*  
*60 K*

SSHADE



Experiment MIR optical constants spectrum of H2O Ia at 15K and Ih at 60K

Spectra

- MIR optical constants spectrum of H2O Ia at 15K
- MIR optical constants spectrum of H2O Ih at 60 K

Sample H2O crystalline ice - deposition 145K - film 0.74µm

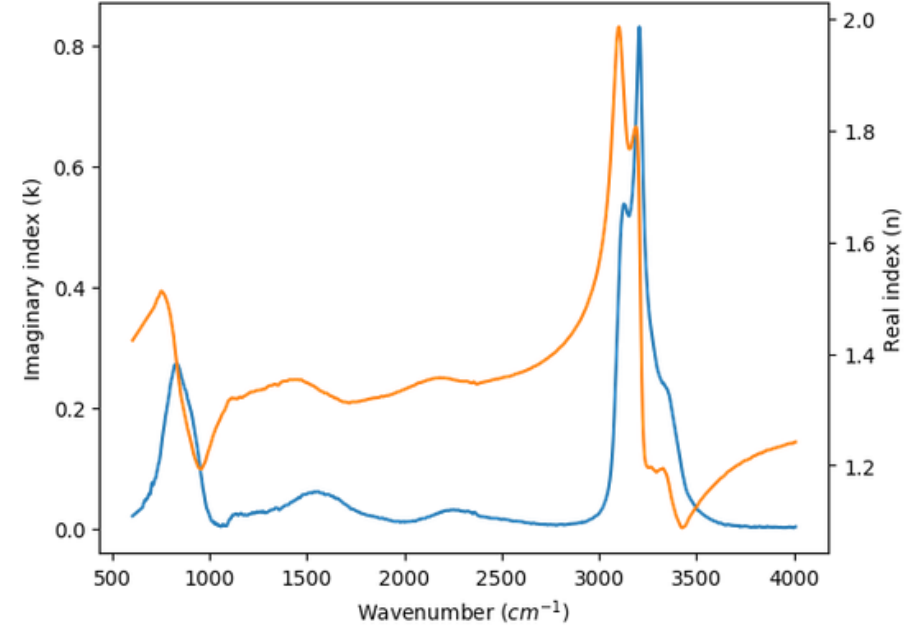
Layer H2O crystalline ice - deposition 145K - film 0.74µm

Material H2O crystalline - phase Ih

Spectrum preview



MIR optical constants spectrum of H2O Ih at 60 K



Title

MIR optical constants spectrum of H2O Ih at 60 K

Database

GhoSST

Spectrum type

optical constants

Version

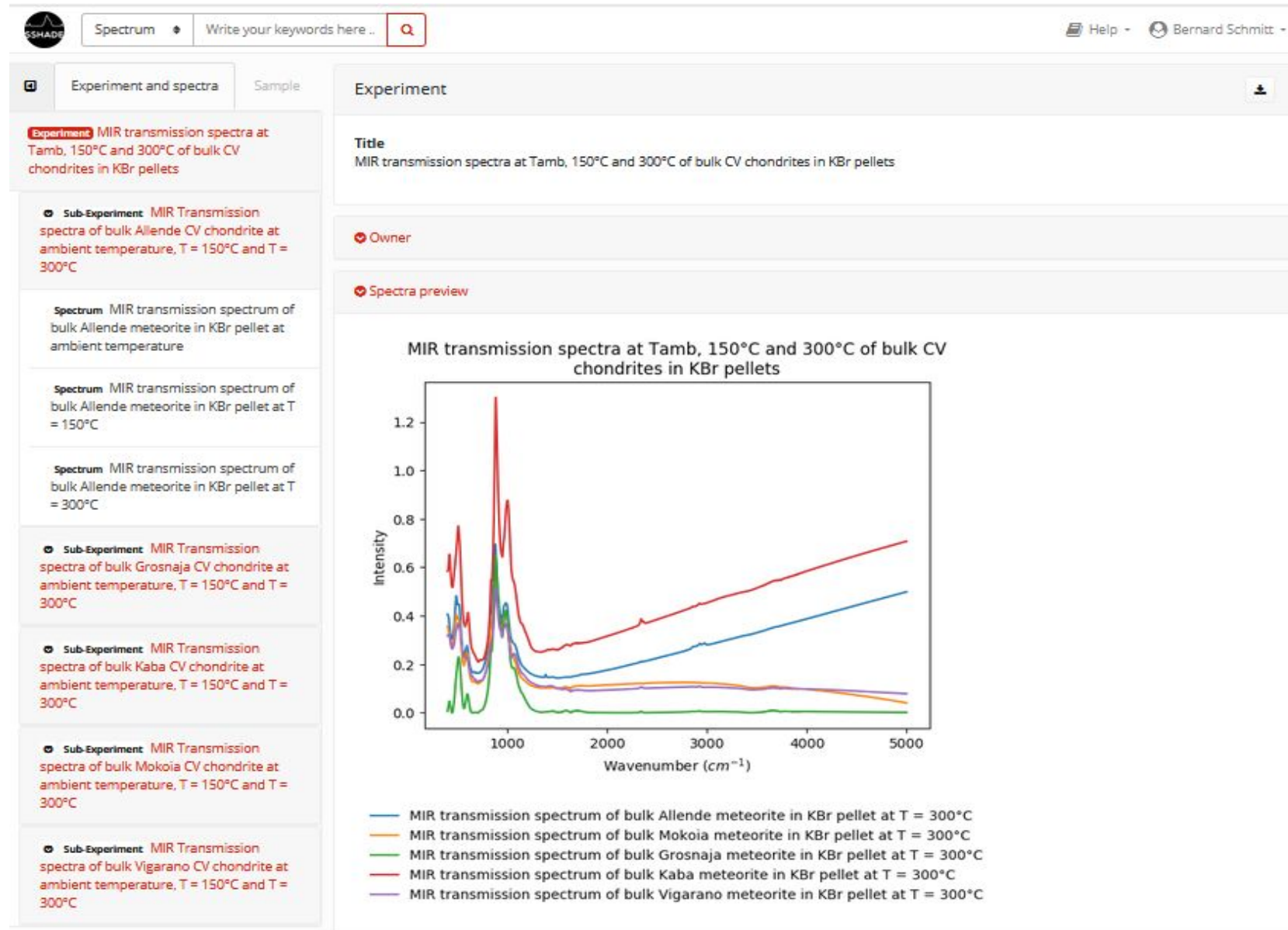
#1 (2017-11-17 17:25:56)

# Examples of SSHADE data

**GhoSST**  
(IPAG – F)

MIR  
Absorbance  
spectra of  
Meteorites

*CV Chondrites*  
20, 150, 300°C





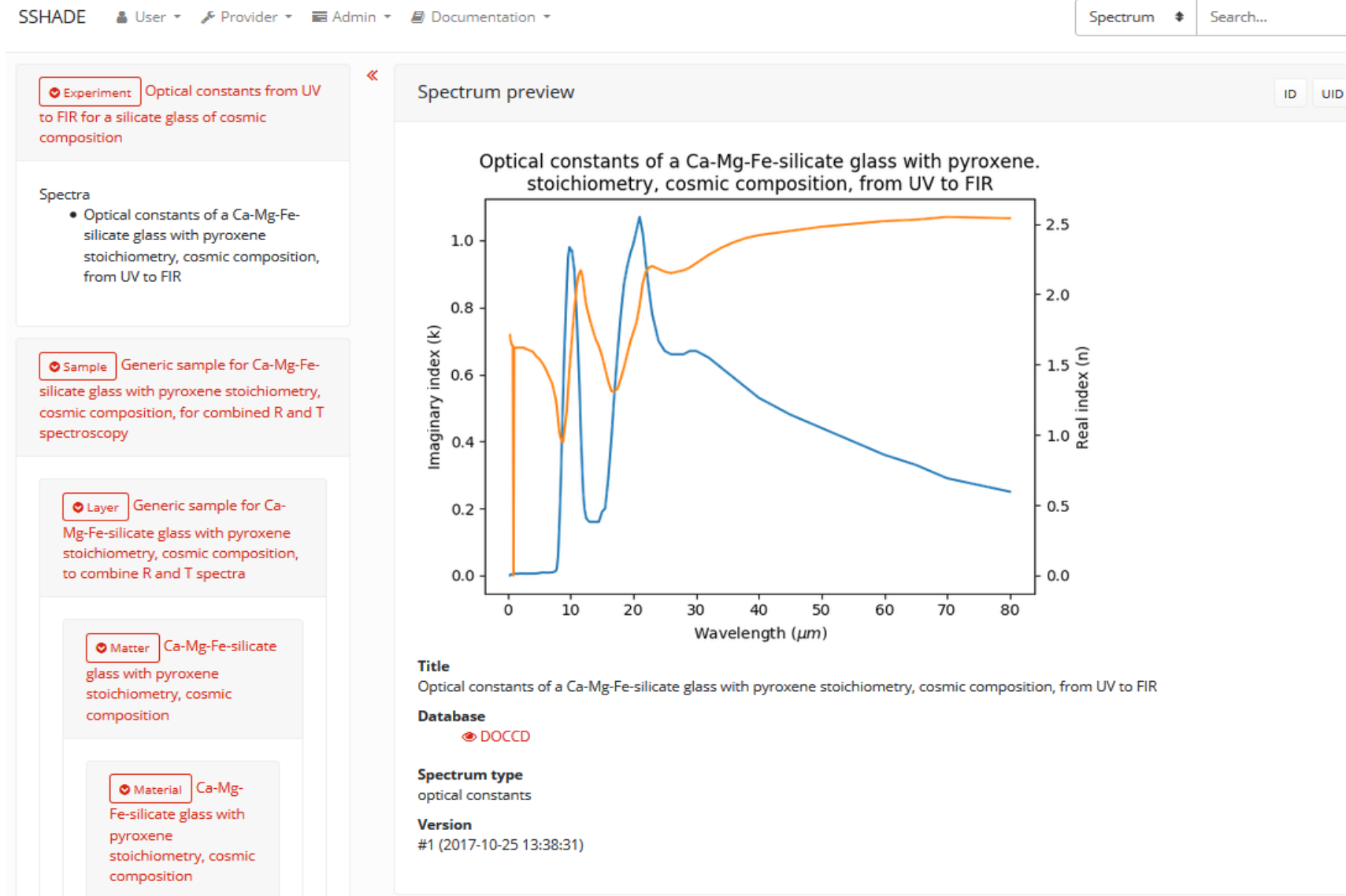
# Examples of SSHADE data

**DOCCD**

(Univ. Jena - D)

UV-FIR  
optical constants  
of minerals

*Ca-Mg-Fe-silicate  
glass with pyroxene,  
cosmic composition*

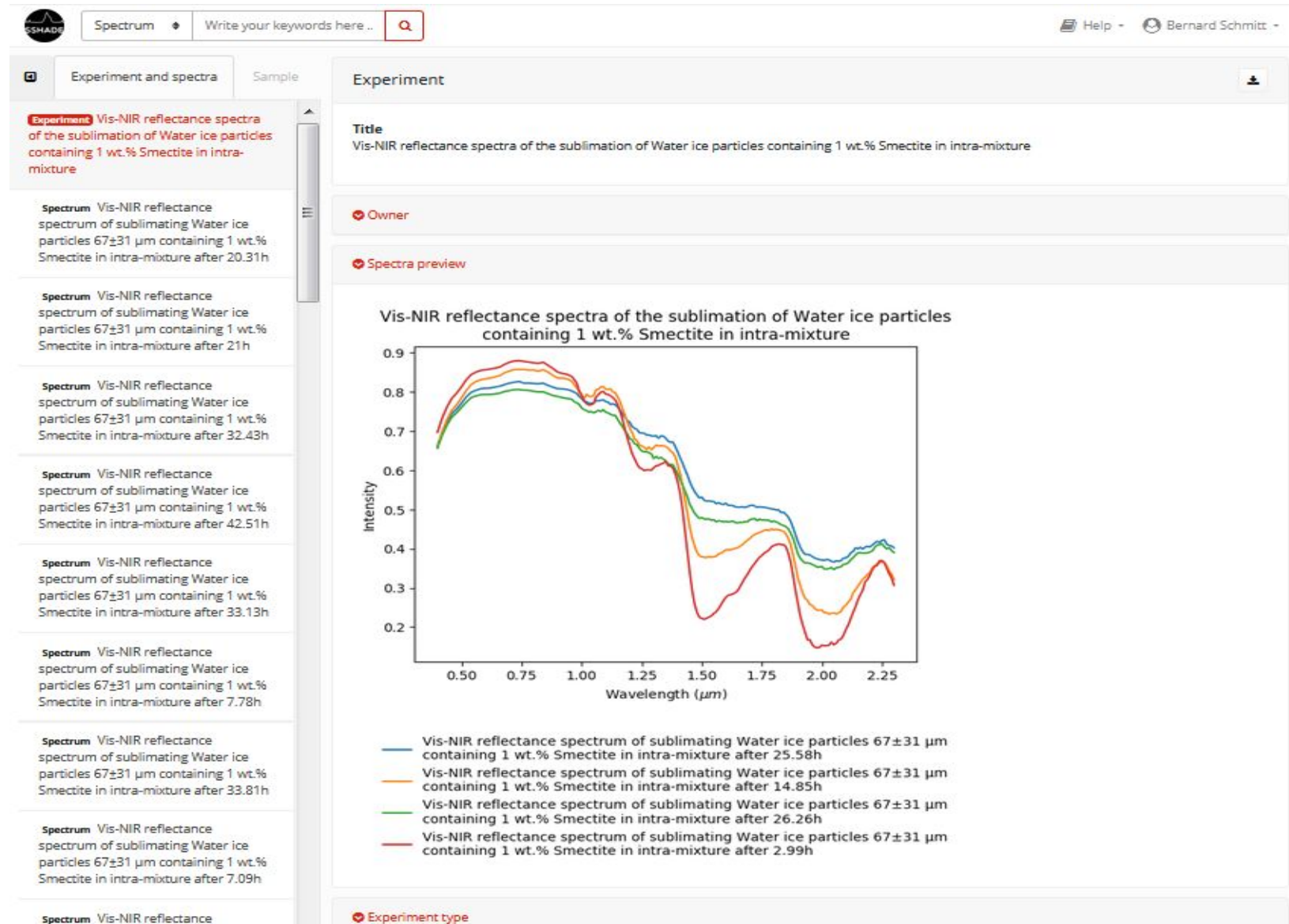


# Examples of SSHADE data

**BYPASS**  
(Univ. Bern)

Reflectance of  
sublimating mixture  
ice-smectite

*99% water ice  
+ 1% Smectite*



# SSHADe Web interface

SSHADe online **1<sup>st</sup> February 2018** at:

<https://www.sshade.eu>

Already in SSHADe:

~ 1400 spectra from > 1000 samples

## SSHADe Web interface

### Search

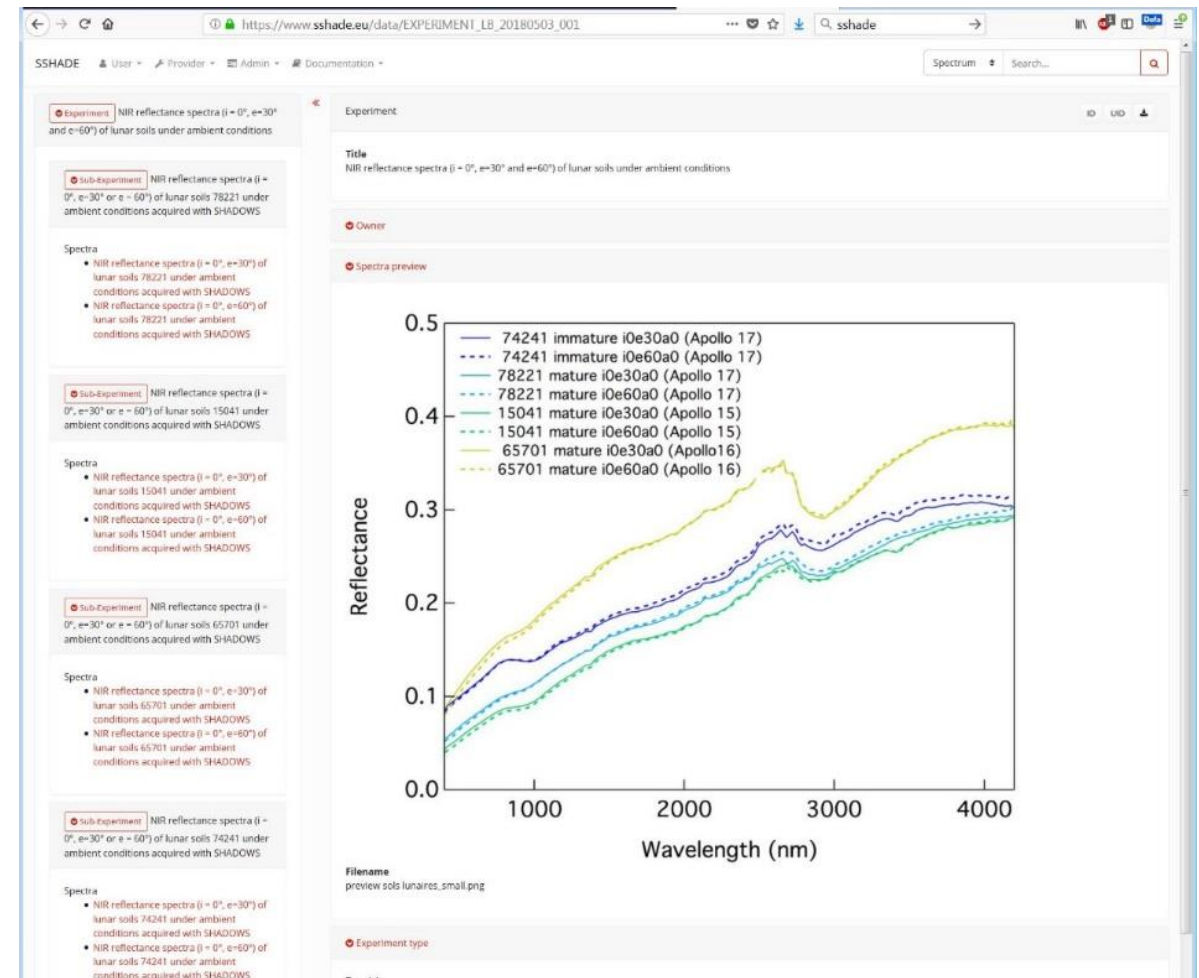
- ✓ Spectra
- ✓ Publications
- ✓ Bandlist

### Visualize

- ✓ Experiment, Spectra
- ✓ Sample details
- ✓ All associated information

### Export

- ✓ Experiment, Spectra
- ✓ Sample details
- ✓ w. links to associated information



# SSHADE Web interface

## Search

- Spectra
- Publications

Provide 2 complementary tools:

- ✓ “Google-style“ toolbar
  - any relevant word
- ✓ Specialized filters

## Spectra

- by experiment,
- by instrument parameters,
- by environment,
- by extra-terrestrial object,
- by sample,
- by composition,
- by publication.

## Publications

- by reference,
- by content,
- by published spectrum

SSHADE User

### Spectra search

optical constants Search Filters Reset

By experiment

By instrument parameters

By environment

By extraterrestrial object

By sample

Sample

Sample name	contains	water ice
Formation mode	contains	condensation
Layer type	in	Granular
Texture	in	Cemented granular, Compact coarse grained, Mixed granular, Loose granular, Sintered granular, Compact fine grained

Materials

Name	contains	H2O ice
Family	in	Snow-ice matter
Origin	in	Laboratory, Natural terrestrial
Reference code	contains	

By composition

By publication

# SSHAE Web interface

## Search results

Spectra fitting the search criteria are displayed either as:

- Spectra (one spectrum of the experiment fits your keyword)
- Experiment (several of its spectra fit)

## Tools:

- **Unfold experiment**  
→ View spectra
- **Quick view**  
→ preview popup
- **Download**  
→ direct or basket

The screenshot shows the 'Spectra search' interface. At the top, there is a search bar containing the keyword 'meteorite'. To the right of the search bar are options for 'in all fields', a 'Filters' button, and a 'Search' button. Below the search bar, it indicates 'Results: 229 spectra'. The results are displayed as a list of items, each with a title and a set of icons for actions like 'View', 'Download', and 'Basket'. The items include:

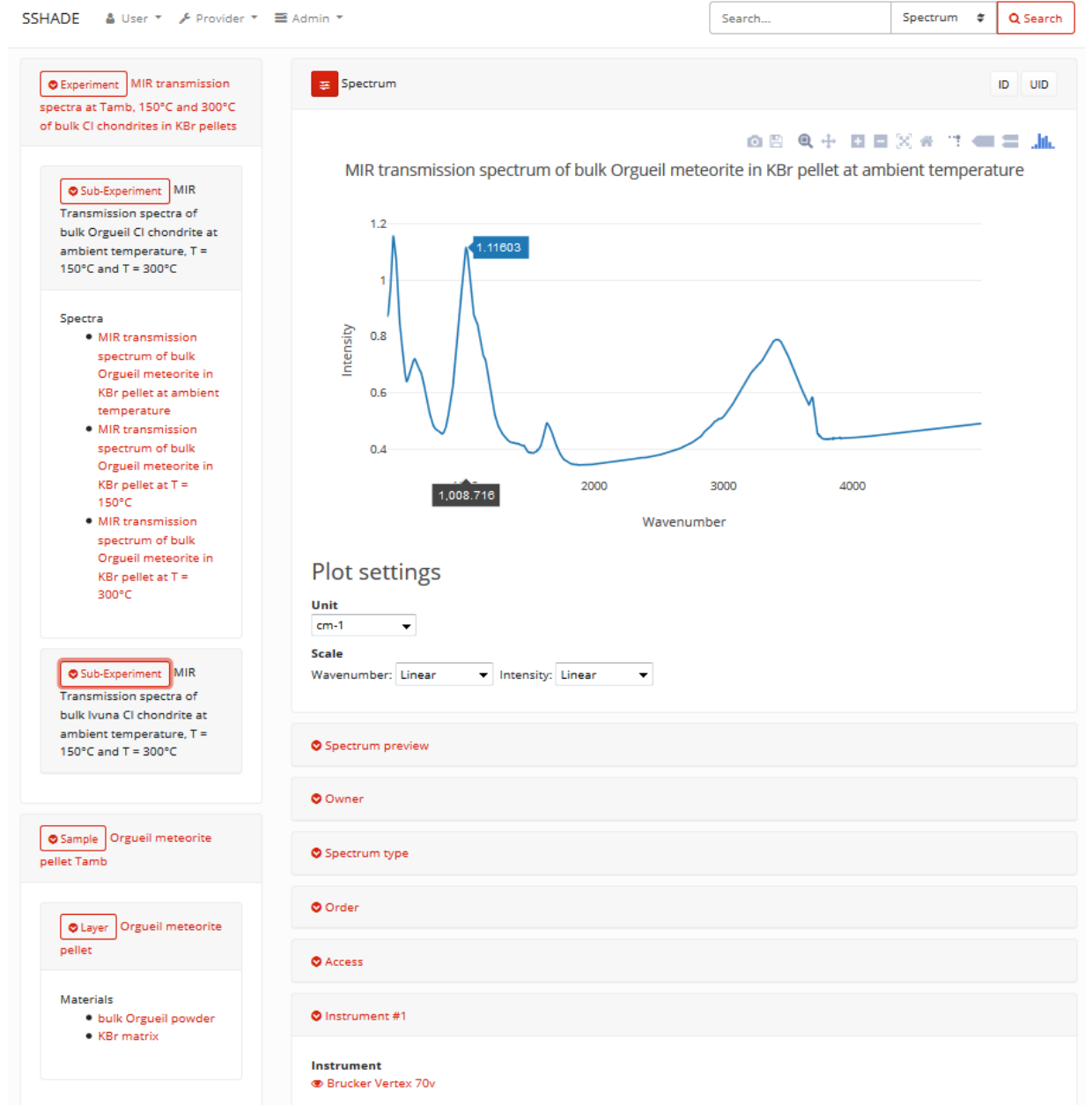
- Averaged Mid-IR spectrum of irradiated Allende pellet ( $Ar^+$ , fluence  $6E15 \text{ ions.cm}^{-2}$ )
- MIR transmission spectrum of bulk EET92002 meteorite in KBr pellet at ambient temperature
- MIR transmission spectrum of bulk ALH85002 meteorite in KBr pellet at ambient temperature
- Averaged Raman spectrum of Murchison pellet 1 irradiated ( $Ar^+$ , fluence  $2E15 \text{ ions.cm}^{-2}$ )
- 15 spectra: MIR transmission spectra at Tamb, 150°C and 300°C of bulk CV chondrites in KBr pellets
- 20 spectra: Raw, normalized and baseline-corrected of MIR transmission spectra of RENAZZO matrix grains pressed on diamonds under vacuum at ambient temperature and 300C
- 19 spectra: Raw, normalized and baseline-corrected of MIR transmission spectra of EET92042 matrix grains pressed on diamonds under vacuum at ambient temperature and 300C
- 10 spectra: Raw, normalized and baseline-corrected of MIR transmission spectra of GRA95229 matrix grains pressed on diamonds under vacuum at ambient temperature and 300C
- 27 spectra: Raw, normalized and baseline-corrected of MIR transmission spectra of QUE99177 matrix grains pressed on diamonds under vacuum at ambient temperature and 300C
- 18 spectra: Raw, normalized and baseline-corrected of MIR transmission spectra of MET00426 matrix grains pressed on diamonds under vacuum at ambient temperature and 300C
- Averaged Raman spectrum of Murchison pellet 2 irradiated ( $Ar^+$ , fluence  $6E15 \text{ ions.cm}^{-2}$ )

# SSHADe Web interface

## Visualize

Provide very complete information on:

- ✓ **Experiment structure and parameters**
  - Spectral, spatial, angular, polarization
  - Instrument used
- ✓ **Spectrum and parameters**



# SSHADe Web interface

## Visualize

Provide very complete information on:

- ✓ **Experiment structure and parameters**
  - Spectral, spatial, angular, polarization
  - Instrument used
- ✓ **Spectrum and parameters**
- ✓ **Sample structure and composition**
  - composition (abundance, ...), texture,
  - physical parameters (T,P, atm...)
  - processes (irradiation...)
  - 'object' (meteorite, micrometeorite, idp...)

The screenshot displays the SSHADe web interface for a sample. At the top, there is a navigation bar with 'SSHADe', 'User', 'Provider', and 'Admin' menus, and a search bar. The main content is divided into two panels. The left panel shows a hierarchical view of the sample structure: 'Sample Orgueil meteorite pellet Tamb' containing a 'Layer Orgueil meteorite pellet' which is composed of 'Materials' including 'bulk Orgueil powder' and 'KBr matrix'. The right panel provides detailed information for the sample, including its name, owner, origin, physical characteristics (thickness, diameter, mass, substrate material), comments, and sample environment parameters (temperature, hydrostatic pressure, fluid type).

SSHADe User Provider Admin

Search... Spectrum Search

Sample Orgueil meteorite pellet Tamb

Layer Orgueil meteorite pellet

Materials

- bulk Orgueil powder
- KBr matrix

Sample

ID UID

**Name**  
Orgueil meteorite pellet Tamb

**Owner of sample**

**Origin of sample**

**Physical characteristics**

**Thickness**  
0.8 ± 0.01 mm

**Diameter**  
13.0 mm

**Mass**  
0.301 ± 0.0015 g

**Substrate material**  
sample holder in aluminium with a centered hole to hold the pellet

**Comments**  
KBr pellet of 13mm of diameter and 0.8mm thick

**Sample environment: Temperature**

**Temperature**  
22.0 ± 2.0 C

**Temperature max**  
22.0 ± 2.0 C

**Sample environment: Hydrostatic pressure**

**Sample environment: Fluid**

**Type**  
vacuum

**Fluid pressure**  
0.001 mbar

**Comments**  
stored in a dessicator

# SSHAE Web interface

## Visualize

Provide very complete information on:

- ✓ **Experiment structure and parameters**
  - Spectral, spatial, angular, polarization
  - Instrument used
- ✓ **Spectrum and parameters**
- ✓ **Sample structure and composition**
  - composition (abundance, ...), texture,
  - physical parameters (T,P, atm...)
  - processes (irradiation...)
  - 'object' (meteorite, micrometeorite, idp...)
- ✓ **Many linked info ! => popups**
  - Publications
  - Documentation, Web sites, ...
  - Minerals, molecules / chemical bonds / atoms

The screenshot displays the SSHAE web interface in a browser. The main page shows a list of experiments with details like 'NIR bidirectional reflection spectra' and 'Smectite SWy-2'. A 'Related data' popup window is open, providing detailed information about an instrument technique. The popup includes the following fields:

- Instrument technique**
- Name:** SHINE Spectro-Gonio Radiometer
- Instrument description**
- Type:** spectro-gonio radiometer
- Name:** SHINE Spectro-Gonio bidirectional reflection Vis-NIR
- Technique:** bidirectional reflection
- Comments:** with series of 6 high pass filters to eliminate high diffraction orders
- Technique description**
- Technique type:** macroscopic
- Source:** Tungsten/Halogen lamp
- Source wavelength:** Vis-NIR
- Source power:** 250 W
- Spectral analyzer(s):** diffraction grating 1200 l/mm - 250nm, diffraction grating 600 l/mm - 400nm, diffraction grating 300 l/mm - 1000nm, diffraction grating 150 l/mm - 4000nm
- Detector(s):** Si, InSb (cryocooler)



# SSHAE Web interface

## Export

### Can export:

- Spectra
- Experiment (several of its spectra fit)

### At different level of the interface

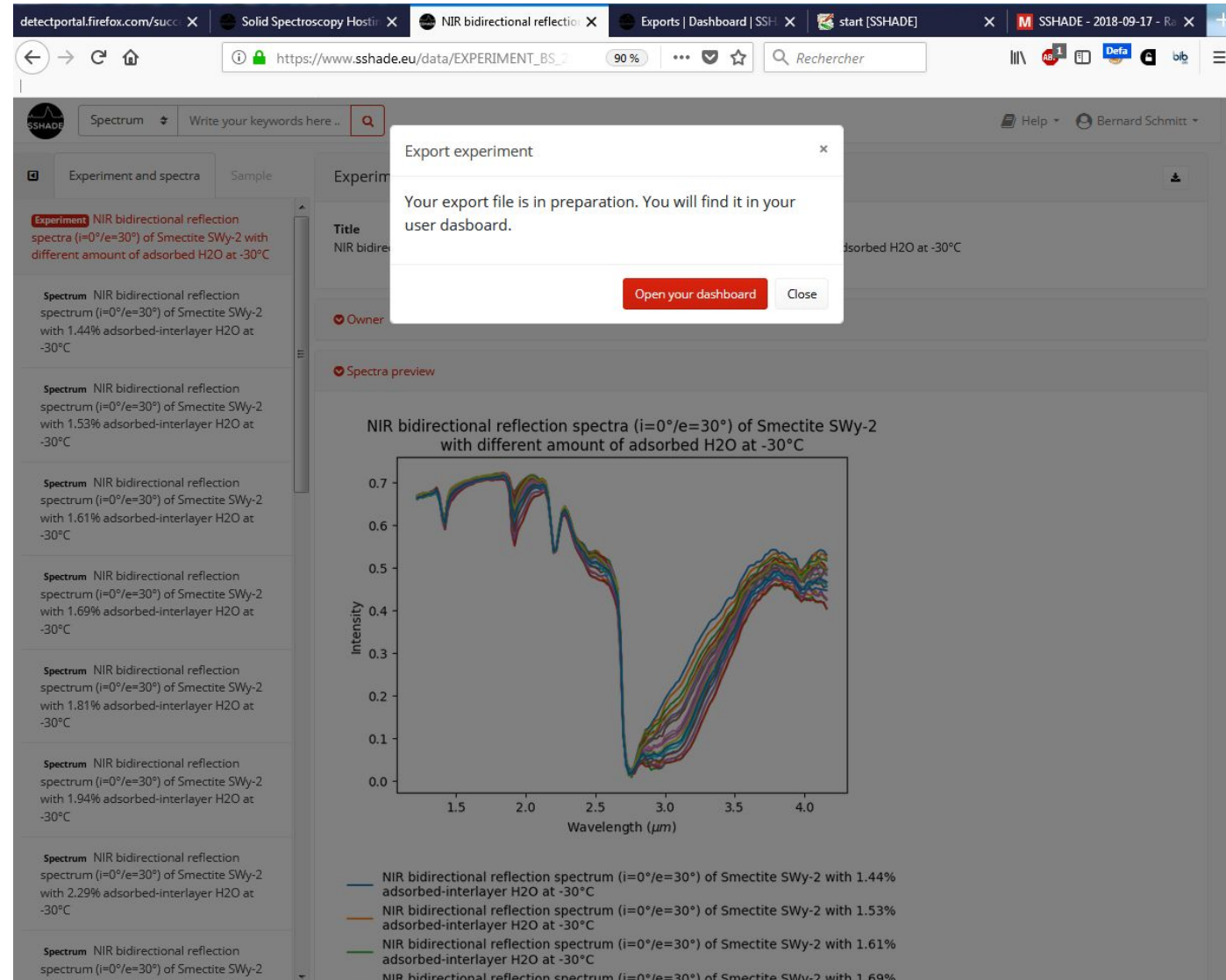
- Search results
- Detail pages of experiment and spectra

### Delivered in a zip file that contains:

- all spectral data
- their experiment and sample metadata
- a 'description' file w. info on spectrum structure & units
- a 'citation file' w. references of the data (paper(s), DOI)

### by asynchronous data extraction:

- stored in dashboard



# SSHADE Web interface

## User dashboard

### Store your download history

- Experiment/Spectra under preparation
  - ➔ download link + share link
- History of your downloads
  - ➔ reload link

The screenshot shows the SSHADE User dashboard. The top navigation bar includes the SSHADE logo, a search bar with the text "Spectrum" and "Write your keywords here ..", and a user profile icon for "Bernard Schmitt". The left sidebar contains a "User" menu with options: Dashboard, Exports (highlighted in red), Imports, Searches, Profile, Data access, and Identity. The main content area is titled "Exports" and contains a table with the following data:

Export	UID	Title	Export date	Size	Steps	Progression	ETA
	SPECTRUM_BS_20130120_003	MIR optical constants spectrum of H2O Ih at 60 K	2018-09-18	465.3 kB	done	<div style="width: 100%;"><div style="width: 100%;"></div></div>	0s
	SPECTRUM_LB_20180326	Vis-NIR bidirectional reflection spectrum ( $i=0^\circ/e=30^\circ/az=0^\circ$ ) of powdered lunar meteorite MAC88105 at 80°C under vacuum	2018-09-18	239.6 kB	done	<div style="width: 100%;"><div style="width: 100%;"></div></div>	0s
	EXPERIMENT_BS_20120803_001	NIR bidirectional reflection spectra ( $i=0^\circ/e=30^\circ$ ) of Smectite SWy-2 with different amount of adsorbed H2O at -30°C	2018-09-17	6.5 MB	done	<div style="width: 100%;"><div style="width: 100%;"></div></div>	0s

## User profile

### Your informations

- Personal
  - Name, login (mandatory)
- Laboratory(ies)

The screenshot shows the SSHADE User profile page. The top navigation bar is identical to the dashboard. The left sidebar has the "Identity" option highlighted in red. The main content area is titled "Identity" and includes a "Change password" button and an "Edit" button. The profile information is as follows:

**E-Mail:** Bernard.P.Schmitt@gmail.com  
**First name:** Bernard  
**Family name:** Schmitt  
**ORCID:** 0000-0002-1230-6627

Below the identity section is the "Laboratories" section, which includes an "Add" button and a table with the following data:

Laboratory name	Organization name	Street	Postal code	City	Region	Country	Description (research topics, ...)
	IPAG	Université Grenoble Alpes - CNRS	122 rue de la Piscine	38400 Saint-Martin d'Hères	Rhône-Alpes	France	laboratory experiments on ices, hydrated minerals and organics. Spectroscopic and hyperspectral remote sensing of icy planetary surfaces (Mars, icy satellites, Pluto,

### Future developments

- Your preferences (search, info,...)

# SSHADE User Wiki

## SSHADE infos

- SSHADE fact sheet
- List of databases and data providers
- [Interface documentation](#)
- SSHADE & SSDM documentation
- Provider documentation (*restricted*)

<https://wiki.sshade.eu>

## User documentation

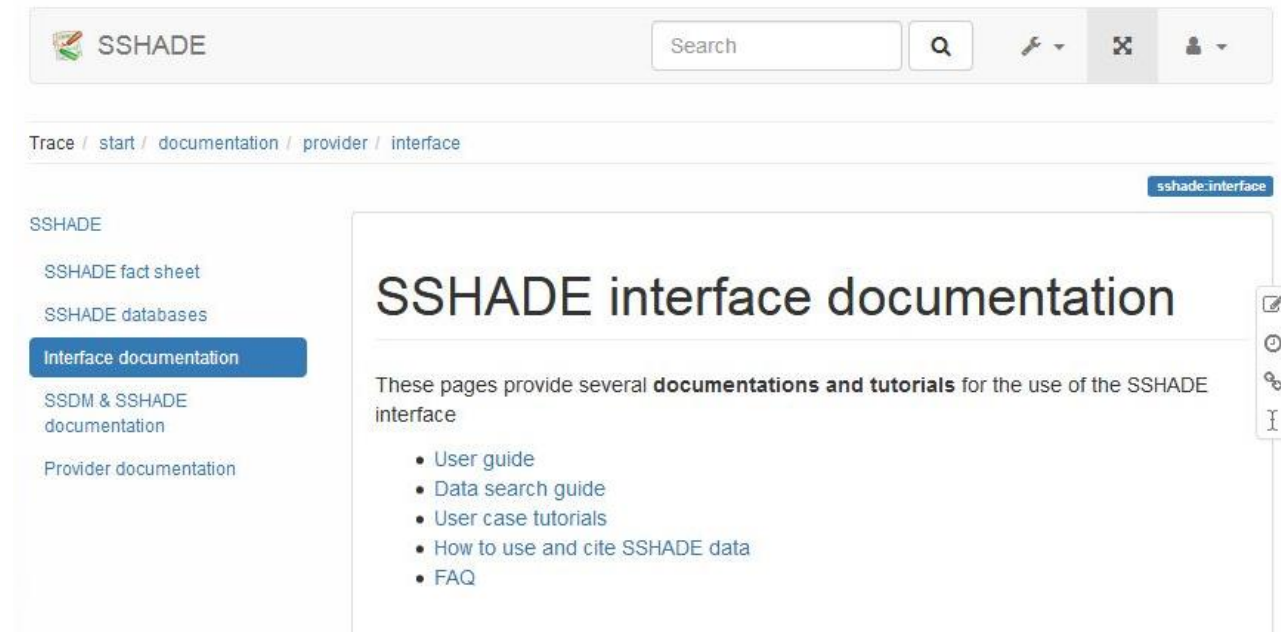
### Interface manuels

- How to login
- How to search spectra & publications
- How to navigate in the interface
- How to export data

### How to use and cite SSHADE data

### Future developments

- User cases videos



The screenshot displays the SSHADE User Wiki interface. At the top, there is a navigation bar with the SSHADE logo, a search box, and utility icons. Below the navigation bar, a breadcrumb trail reads 'Trace / start / documentation / provider / interface'. The main content area is divided into a left sidebar and a main panel. The sidebar lists several documentation topics: 'SSHADE fact sheet', 'SSHADE databases', 'Interface documentation' (which is highlighted with a blue background), 'SSDM & SSHADE documentation', and 'Provider documentation'. The main panel features the title 'SSHADE interface documentation' and a sub-header 'These pages provide several **documentations and tutorials** for the use of the SSHADE interface'. Below this, a list of links is provided: 'User guide', 'Data search guide', 'User case tutorials', 'How to use and cite SSHADE data', and 'FAQ'. A vertical toolbar with various icons is visible on the right side of the main panel.

# Future developments: 2018-2019

## Band list : bands and states

List of band positions, width, intensity, transition modes ... of a solid constituent in a defined environment (T, P, composition, phase, ...)

- Bands parameters
  - position (energy), width, shape, ...
  - intensities (peak and integrated)
  - accuracies / quality / evaluation
- Transitions assignment
  - states QN, anharmonic coefficients, ...
- Search/Display/Export interface
  - Search specific band (position, composition, ...), display/export list of bands

## VO interoperability

- With VESPA: in process of finalization in Europlanet-2020 RI
- With VAMDC: first need extension of XSAMS datamodel (planned)