EUROPLANET 2020-RI - VESPA WP

European Data Bases Infrastructure of Solid Spectroscopy

SSHADE

Solid Spectroscopy Hosting Architecture of Databases & Expertise

https://www.sshade.eu

Bernard Schmitt, Philippe Bollard, Alexandre Garenne,
Damien Albert, Lydie Bonal and the SSHADE Consortium Partners

The SSHADE database infrastructure

for Astrophysics, Planetary sciences and Geosciences

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

GhoSST

FAME

LayeredSilicatesDatabase

BYPASS Bern icY Planetary Analogues ...

in the **electromagnetic spectrum**

From a Consortium of laboratories

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

SSHADE European Consortium of Data Providers

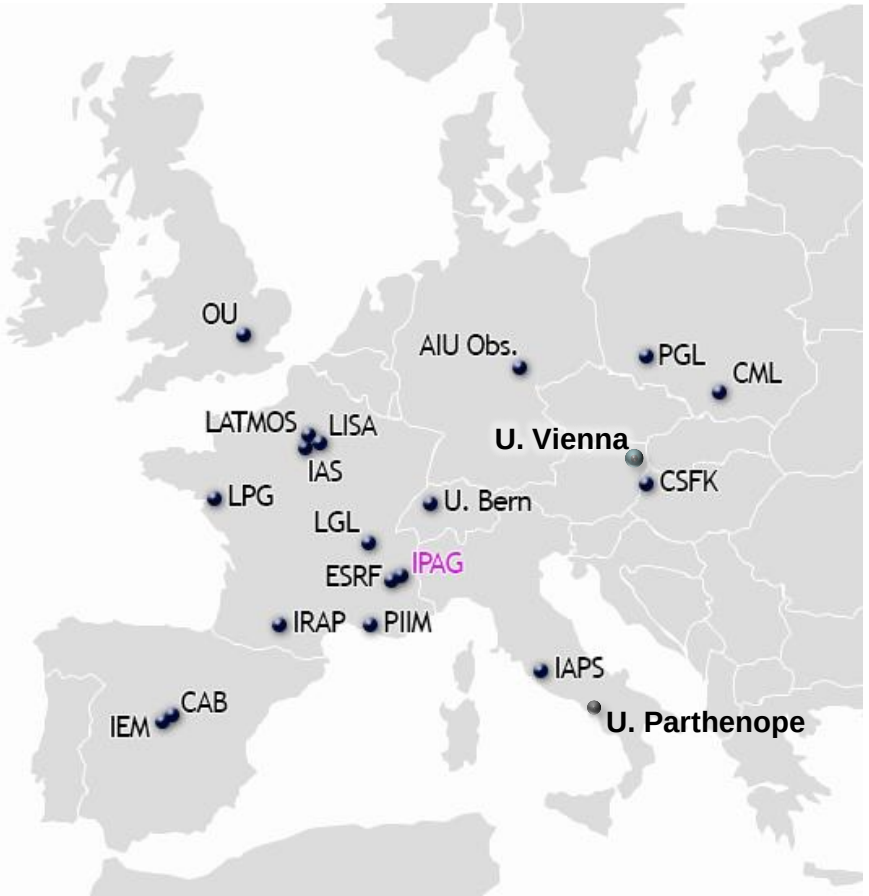
Data from **23** solid spectroscopy experimental groups
in **8** European countries (F, PL, D, GB, CH, E, I, HU) +India +Taiwan
~**75** researchers

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*

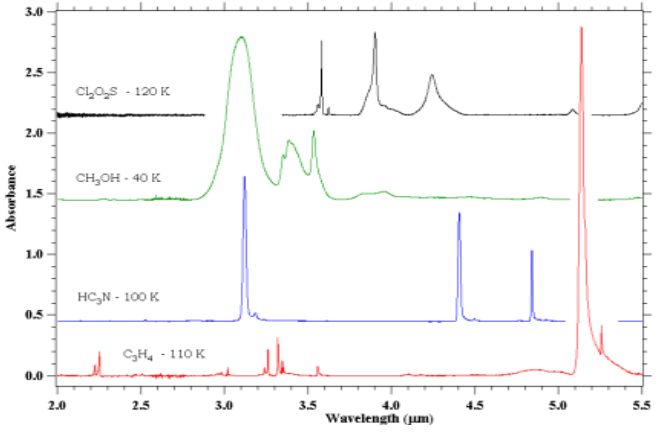
- **Provide to the planetary and astrophysics community**
  - **Spectral and spectro-photometric data**
    - over all the electromagnetic spectrum
    - on all types of solid materials (but also liquid)
    - from synthetic, terrestrial or extraterrestrial samples
  - **With well documented information**
    - 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* ?

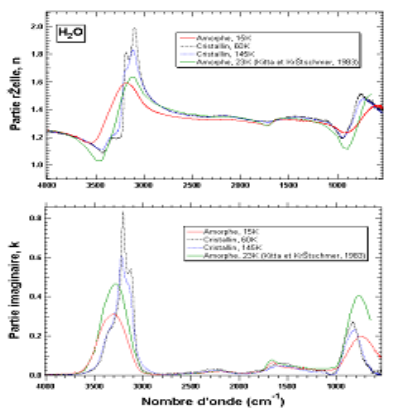
- **Materials**
  - **Ices** (low/high T-P, mixtures, ...), molecular solids, snow…
  - **Minerals,** rocks
  - **Organic solids,** polymers, **Carbonaceous materials,** …
  - **Inorganic solids**, Metals, …
  - also some **liquids**

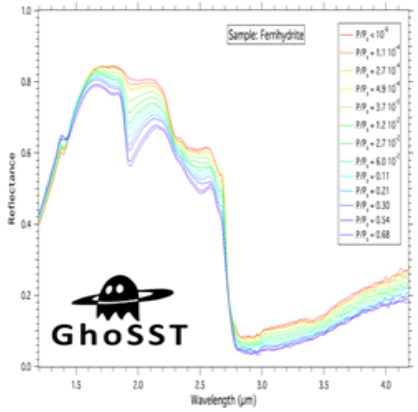


- **Samples**
  - **Synthesized** in the laboratory
  - **Natural terrestrial analogues** collected or measured in the field
  - **Cosmomaterials collected on Earth**: (micro-)meteorites, *IDPs,* …
  - **Extra-terrestrial samples** collected on planetary bodies: lunar soils…

Which types of spectra in *SSHADE* ?

- **Spectral ranges:**
  - Designed from g-rays to radio wavelengths
  - Now mostly **from near-UV to sub-mm (0.3µm - 1mm),** plus **X-rays**.





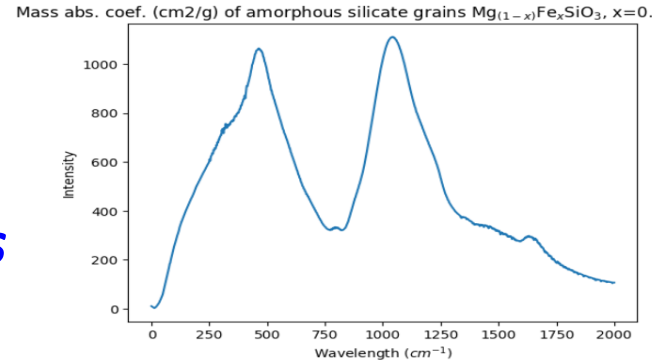
- **Types of data:**

➢ **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***

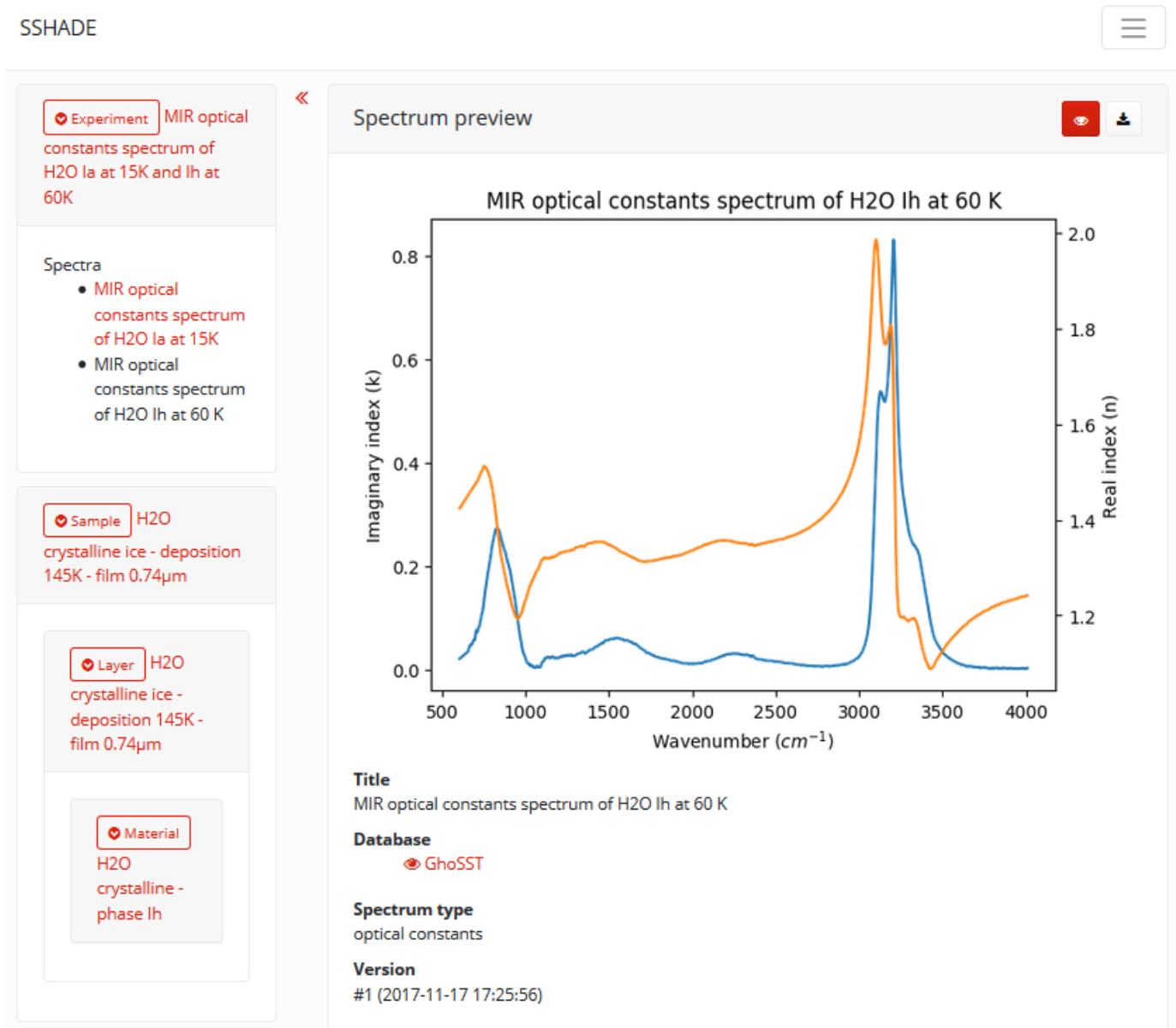


Examples of SSHADE data

GhoSST
(IPAG – F)

MIR-FIR
optical constants
of ices

H_2O ice crystalline
60 K

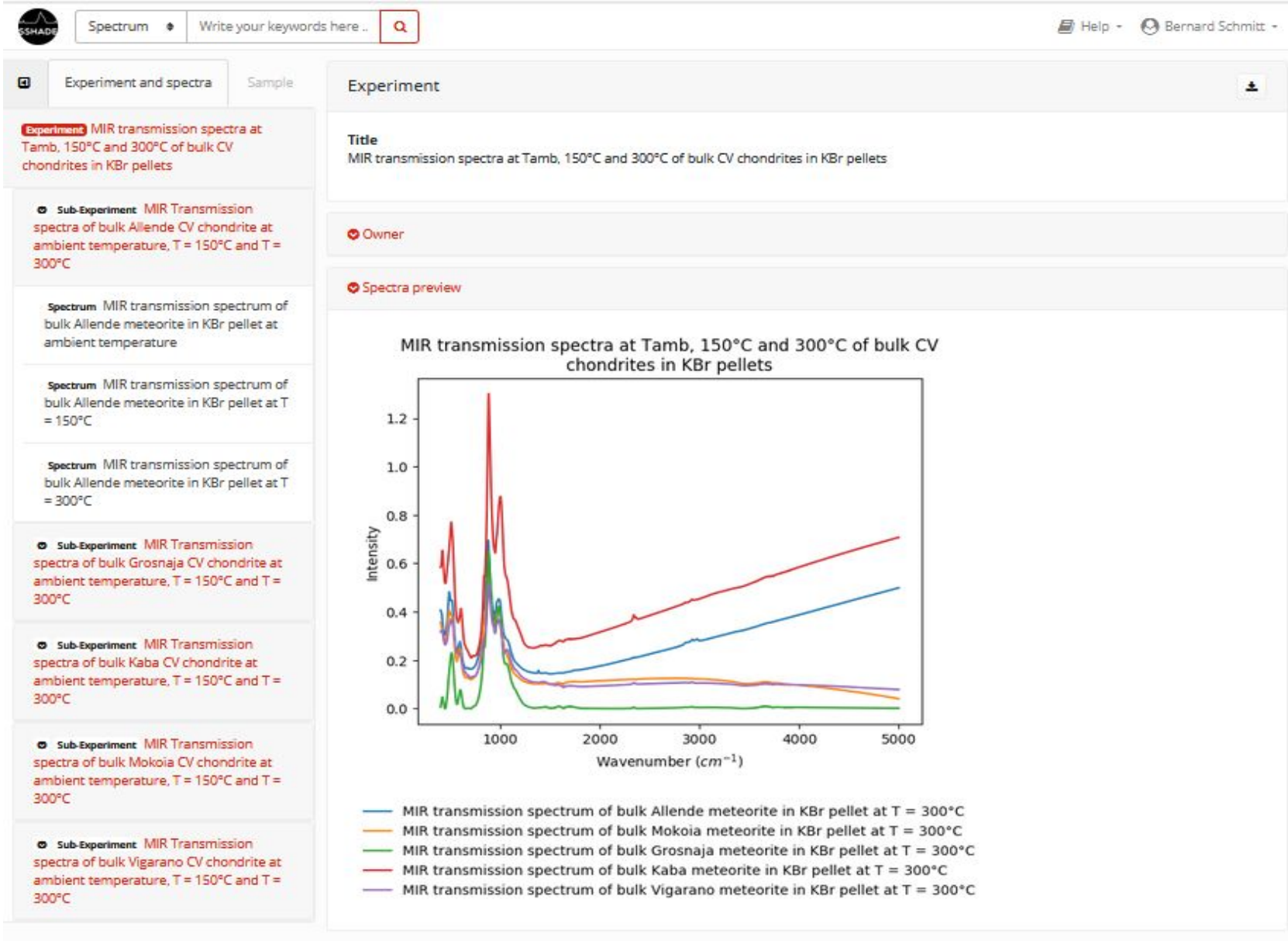


Examples of SSHADE data

GhoSST
(IPAG – F)

MIR
Absorbance
spectra of
Meteorites

CV Chondrites
20, 150, 300°C

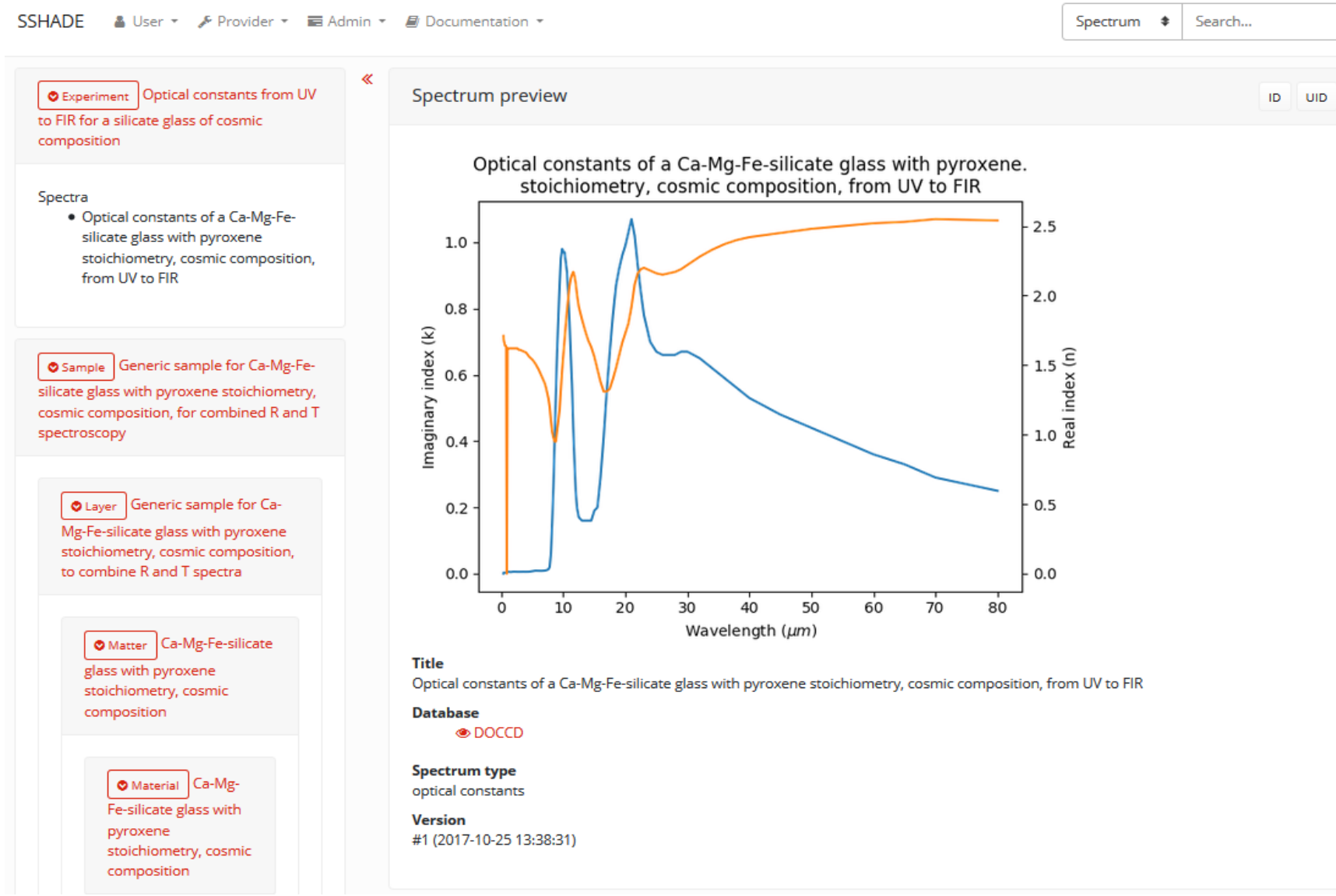


Examples of SSHADE data

DOCCD
(Univ. Jena - D)

UV-FIR
optical constants
of minerals

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

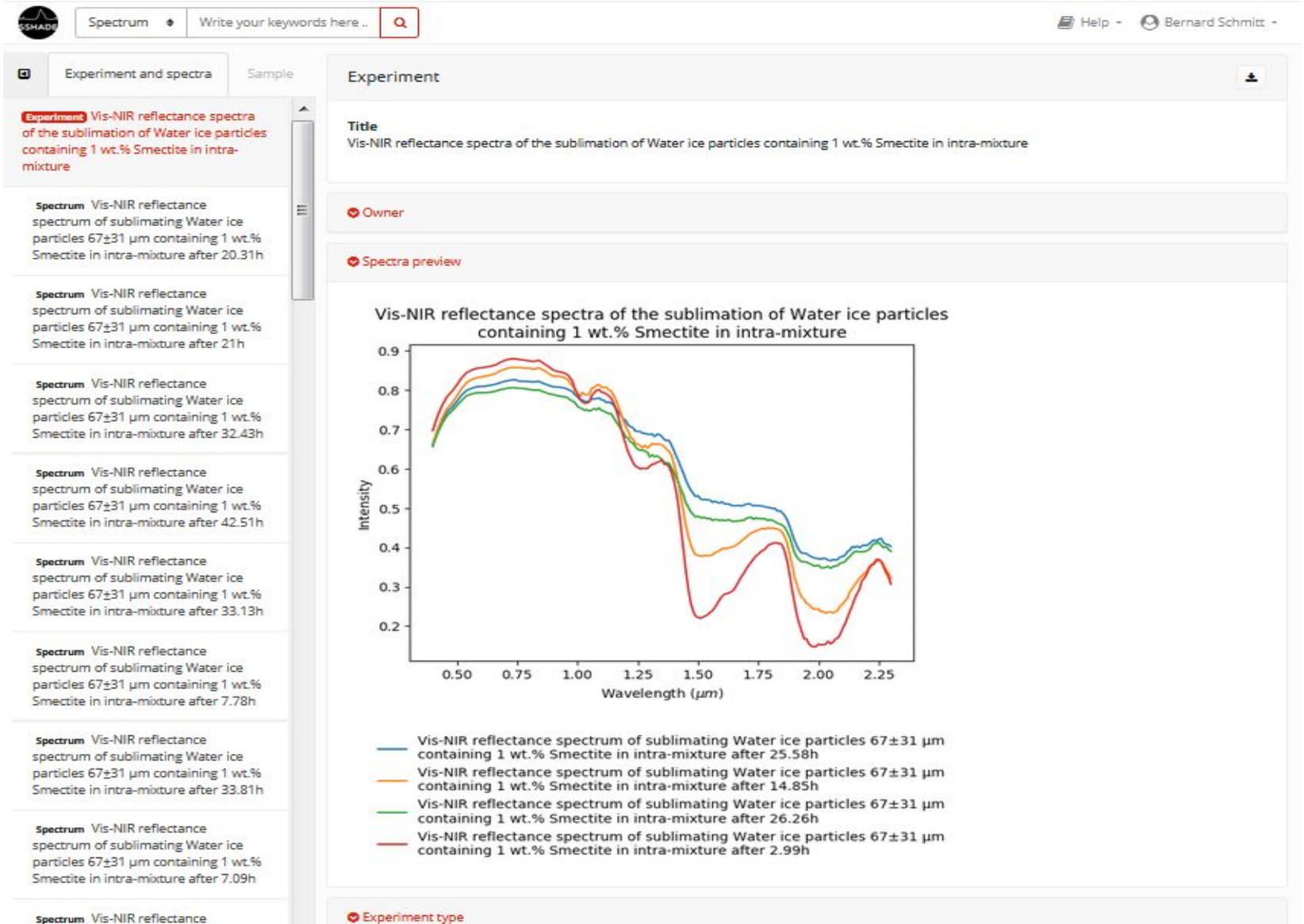


Examples of SSHADE data

BYPASS
(Univ. Bern)

Reflectance of sublimating mixture ice-smectite

99% water ice
+ 1% Smectite



SSHADE Web interface

SSHADE online 1st February 2018 at:

https://www.**sshade.eu**

SSHADE Web interface

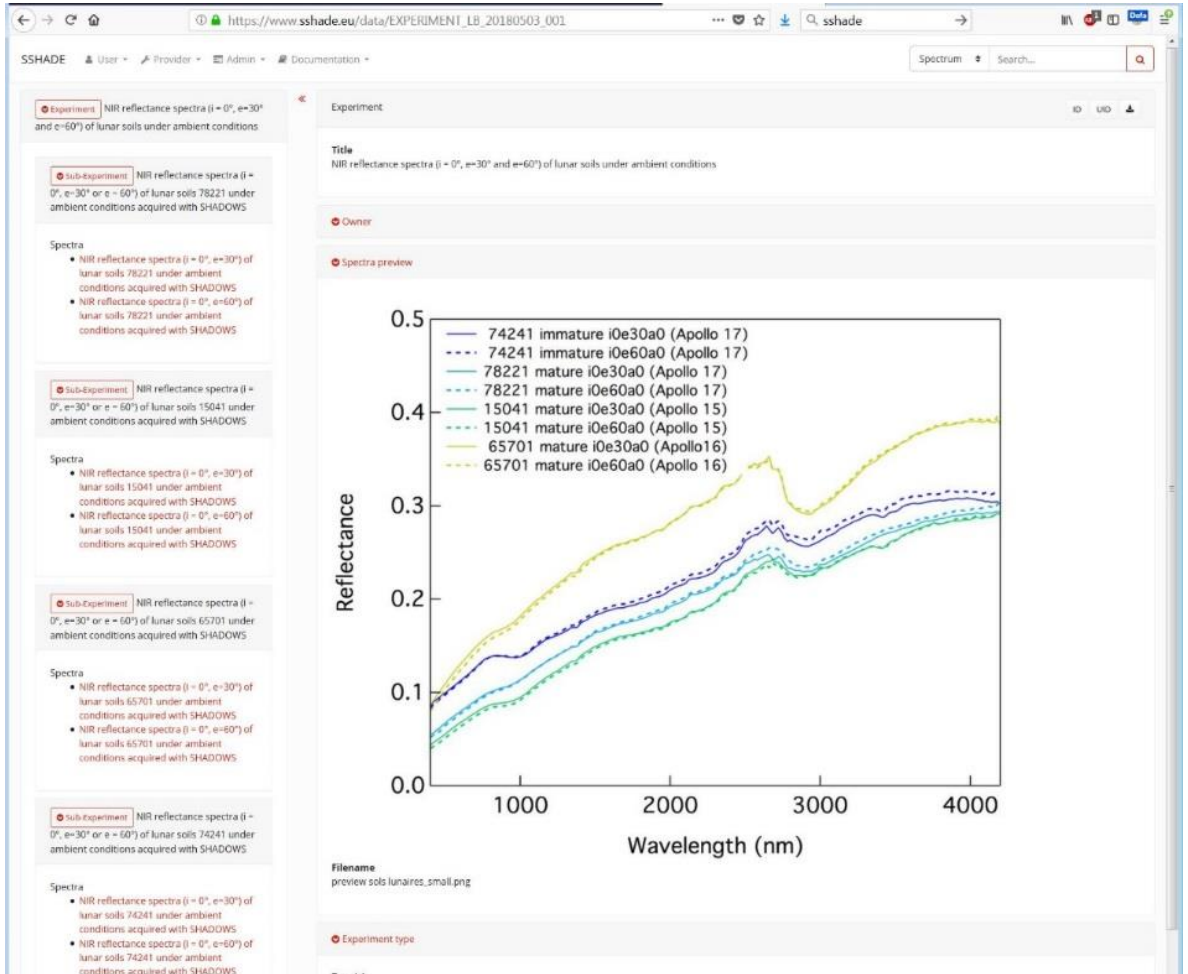
Search
- ✓ **Spectra**
- ✓ **Publications**
- ✓ **Bandlist**

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

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

Already in SSHADE:

~ 1400 spectra from > 1000 samples



SSHADE Web interface

Search

- **Spectra**
- **Publications**

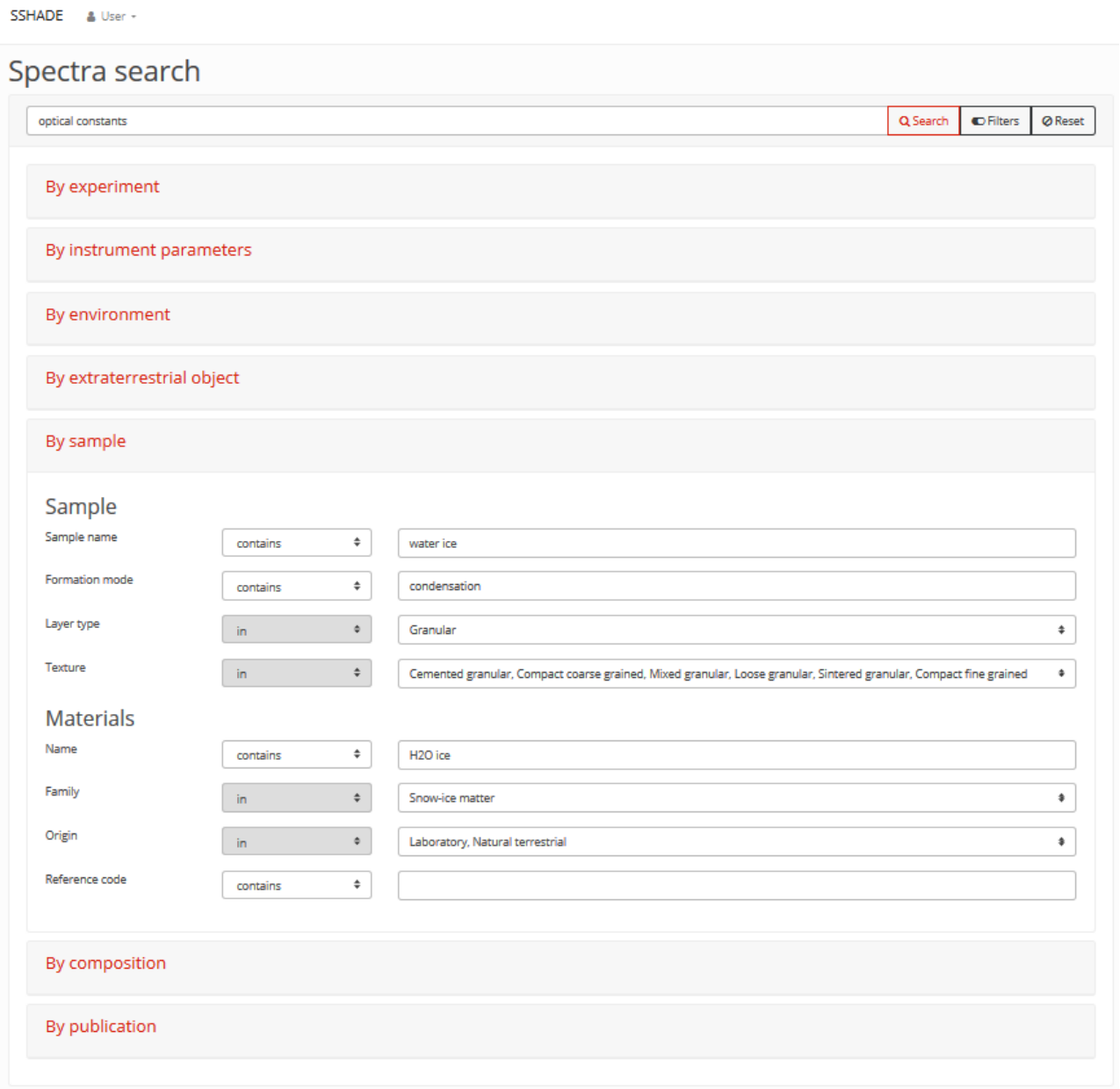
Provide 2 complementary tools:

✓ **“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 Web interface

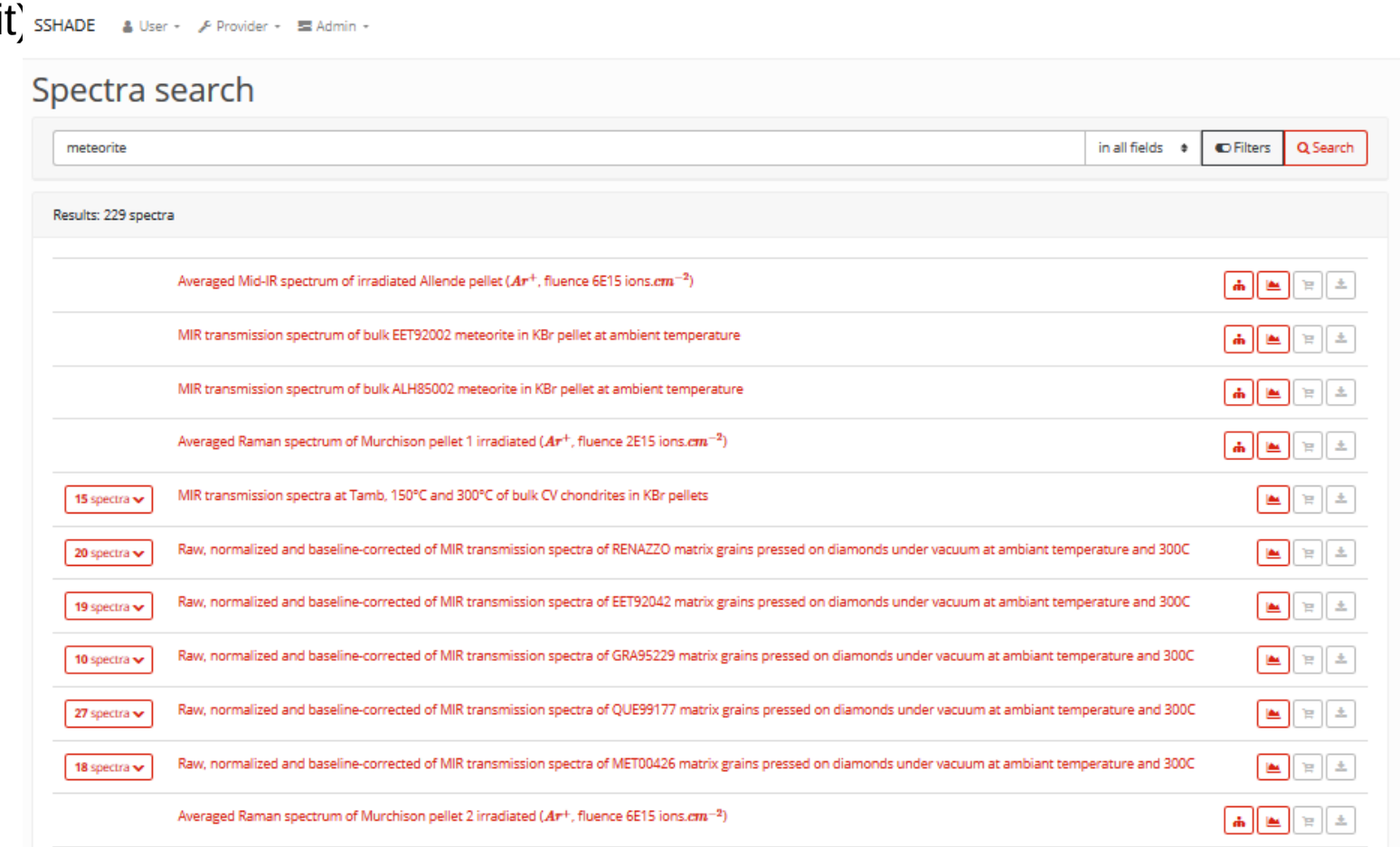
Search results

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

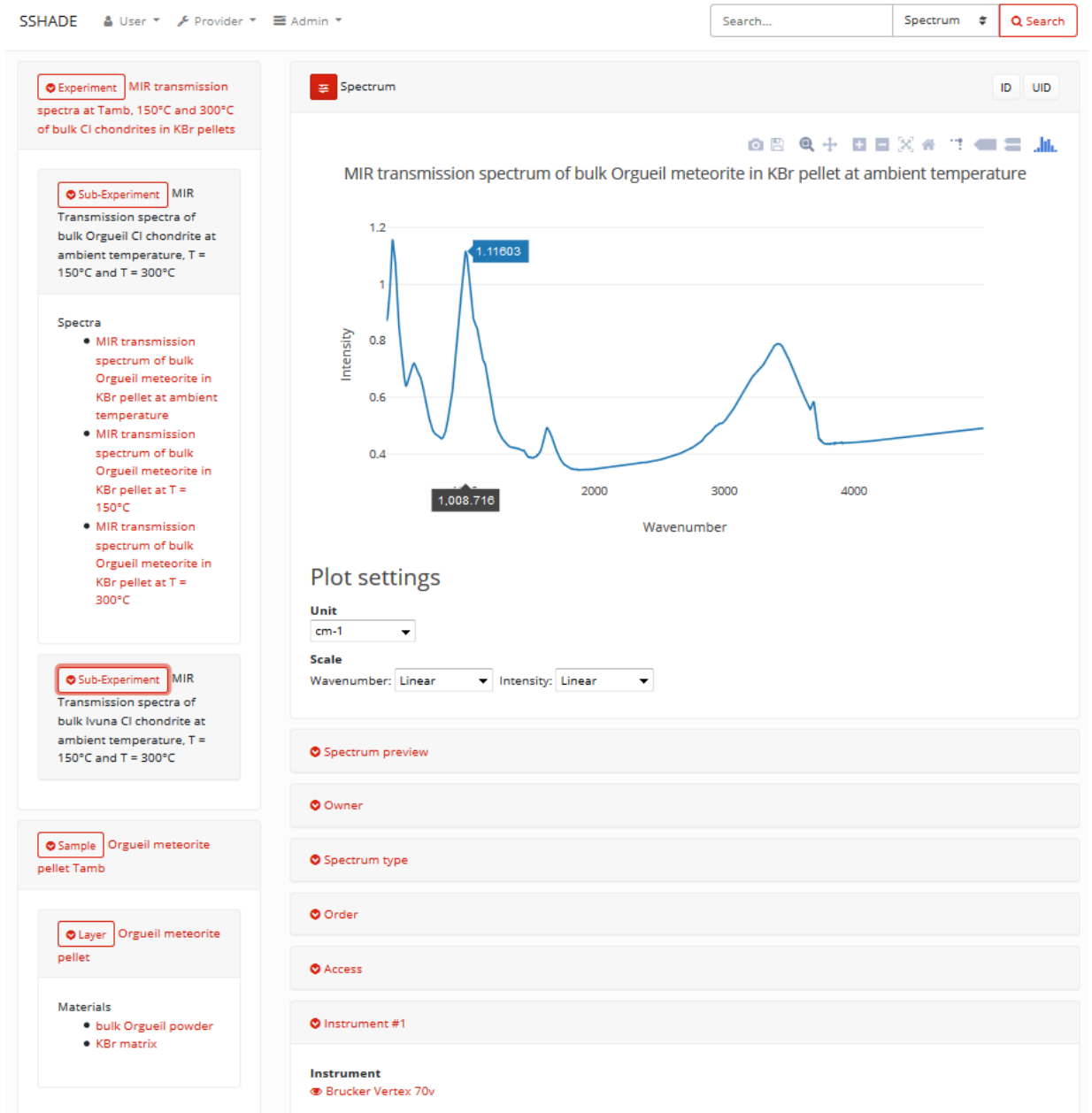


SSHADE Web interface

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:

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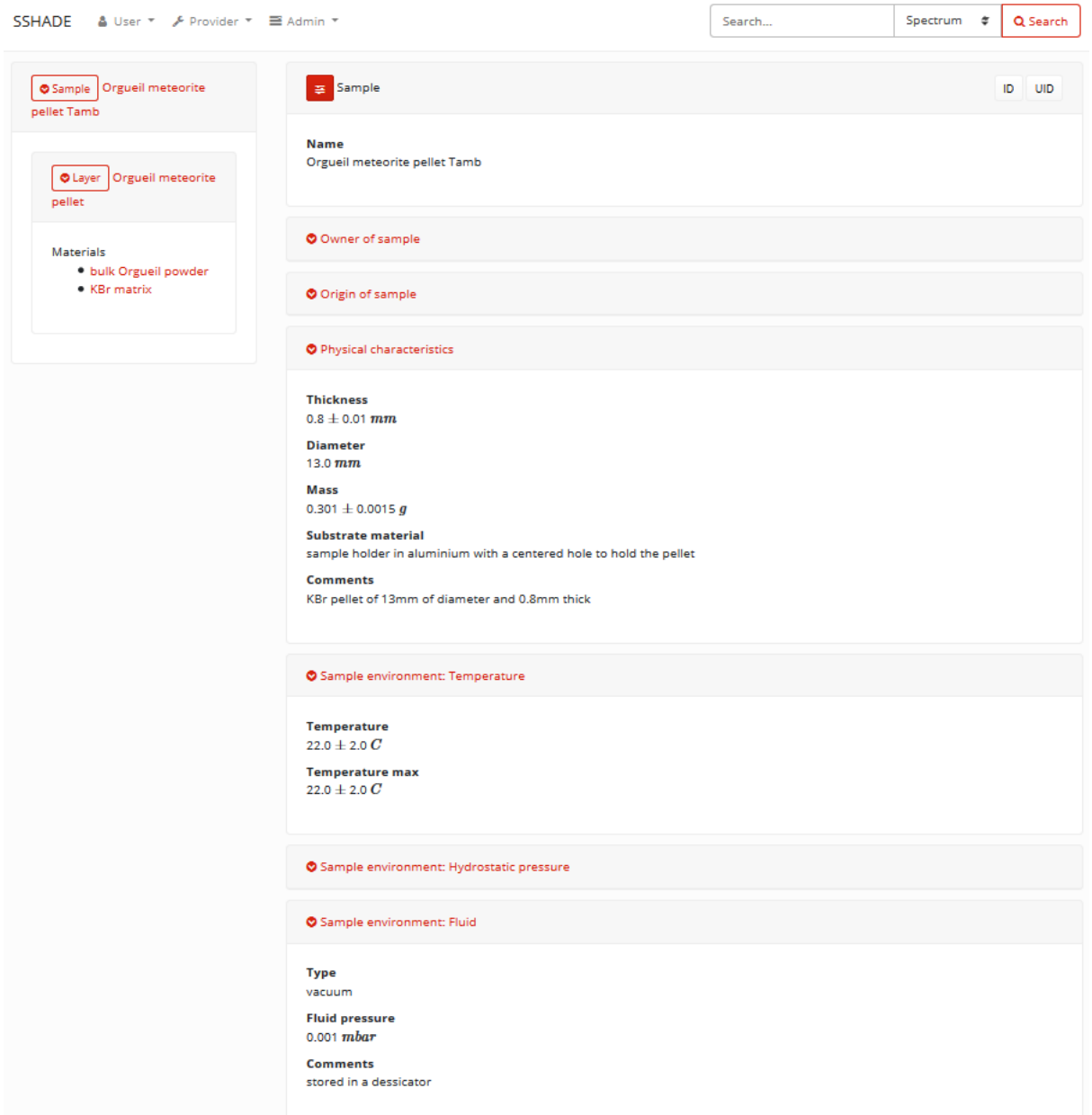
  - ➢ Instrument used
- ✓ **Spectrum and parameters**
- ✓ **Sample structure and composition**
  - ➢ composition (abundance, …), texture,
  - ➢ physical parameters (T,P, atm…)
  - ➢ processes (irradiation…)
  - ➢ ‘object’ (meteorite, micrometeorite, idp…)



SSHADE Web interface

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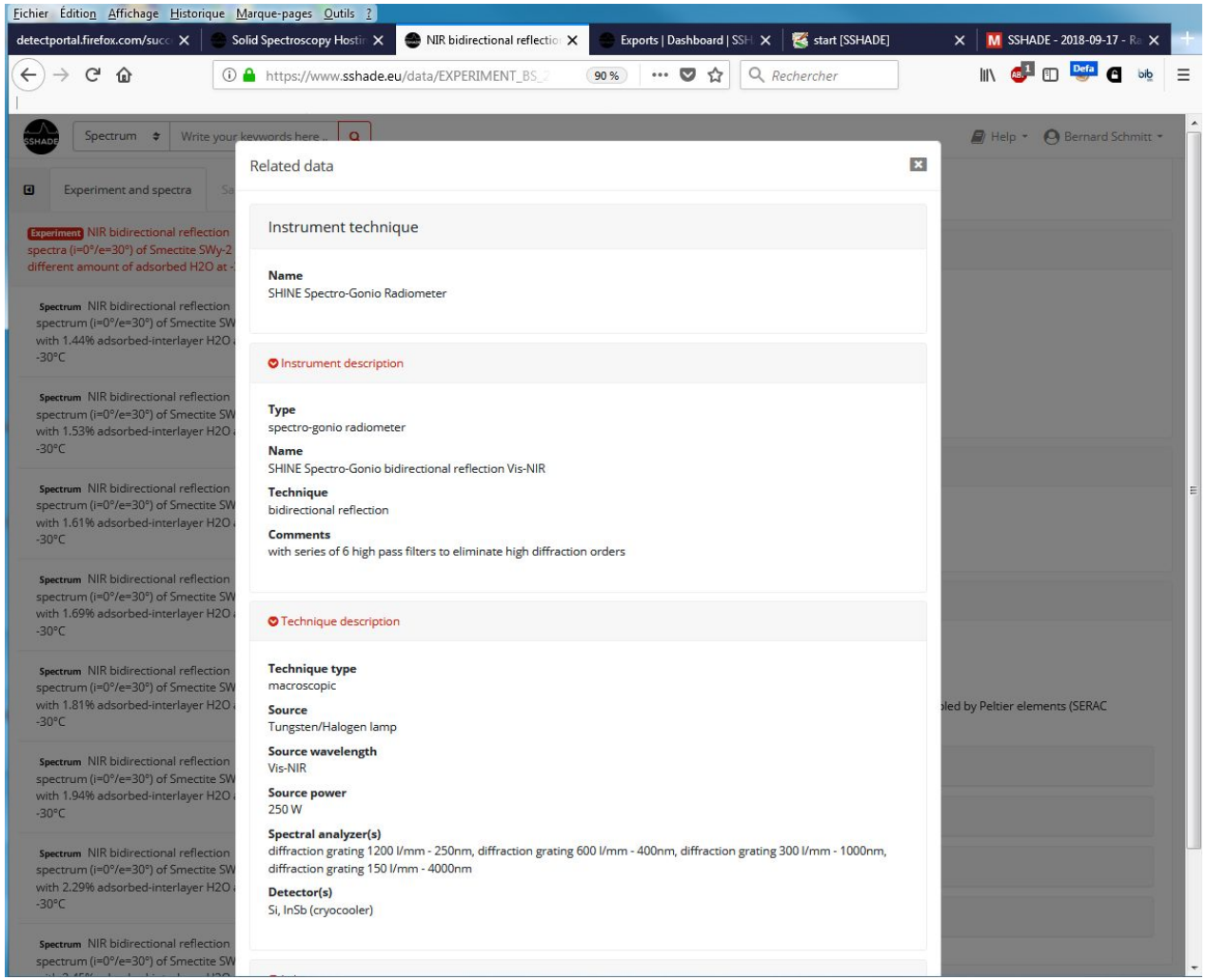
  - ➢ processes (irradiation…)
  - ➢ ‘object’ (meteorite, micrometeorite, idp…)
- ✓ **Many linked info ! => popups**
  - ➢ Publications
  - ➢ Documentation, Web sites, …
  - ➢ Minerals, molecules / chemical bonds / atoms



SSHADE Web interface

Export

Can export:

- Spectra
- Experiment (several of its spectra fit)

At different level of the interface

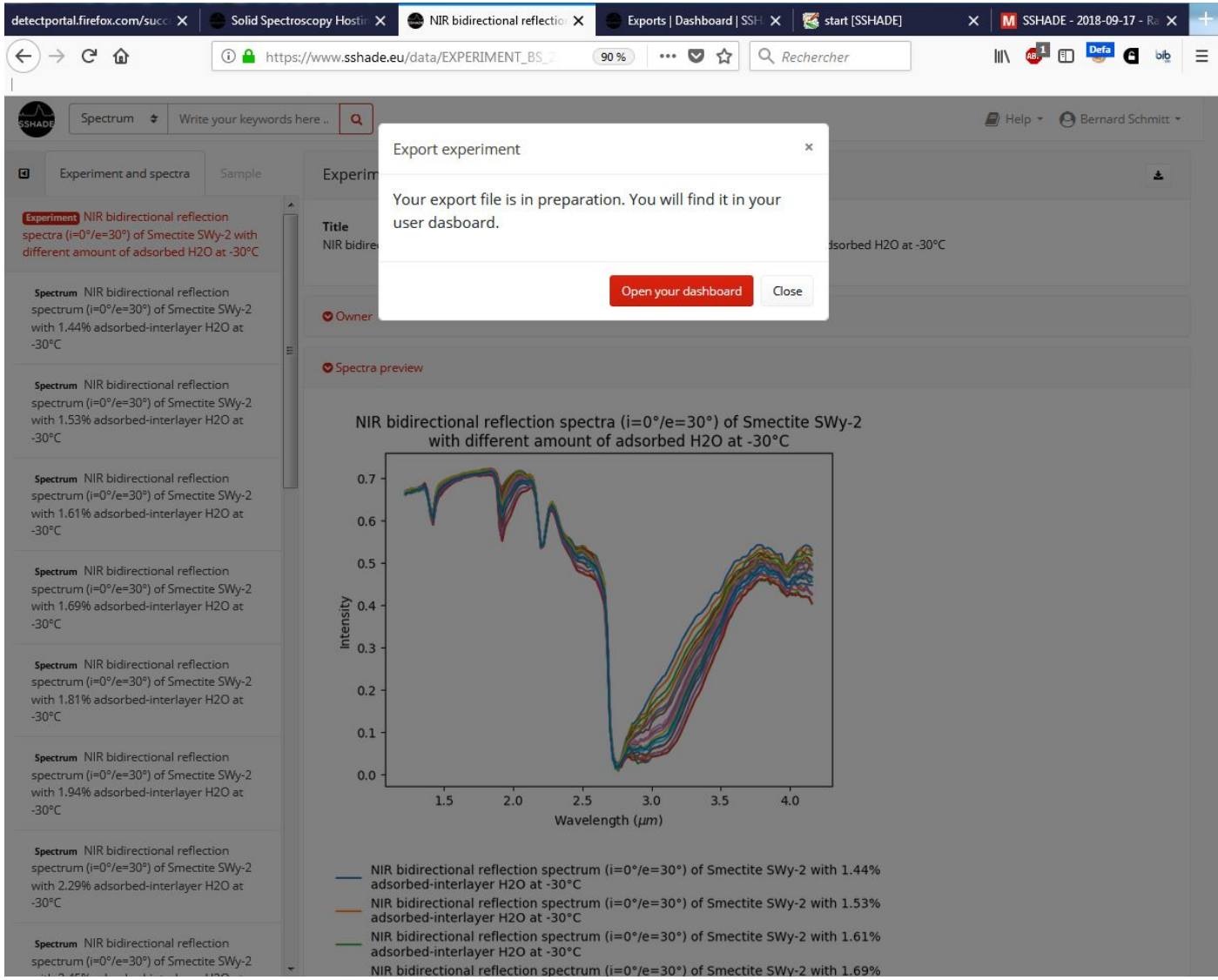
- Search results
- Detail pages of experiment and spectra

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

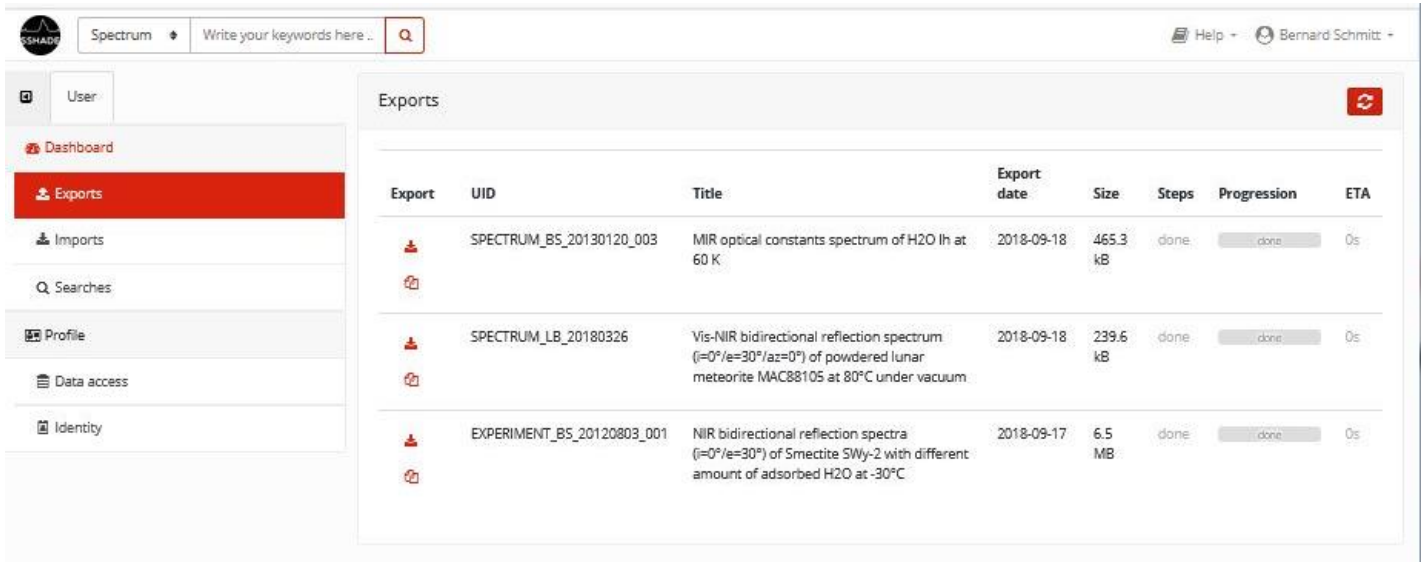
Store your download history

- Experiment/Spectra under preparation

  ➔ download link + share link

- History of your downloads

  ➔ reload link



User profile

Your informations

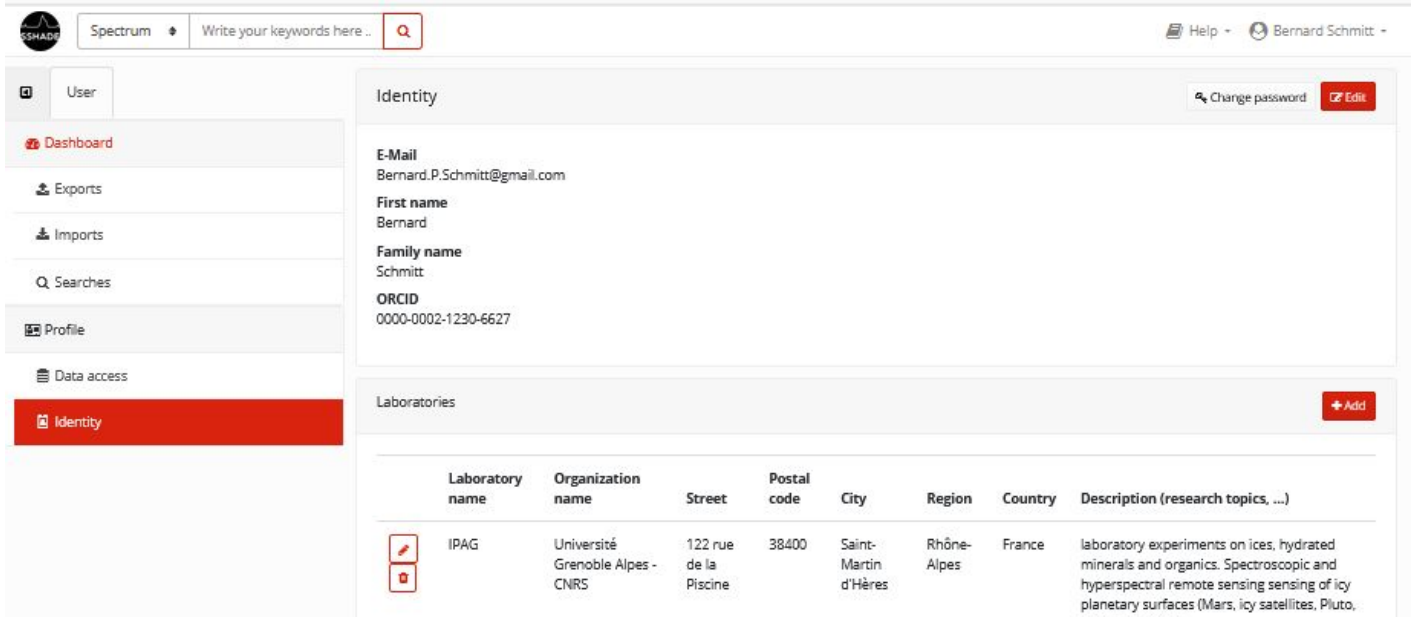
- Personal

  Name, login (mandatory)

- Laboratory(ies)

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

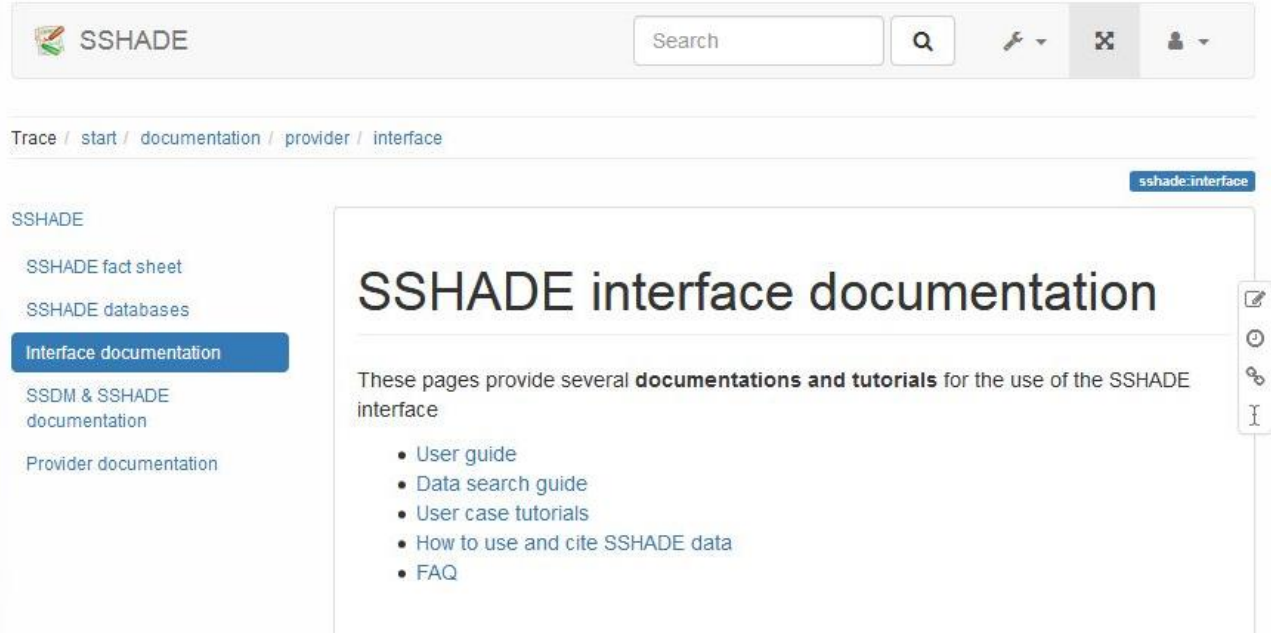
Interface manuels

- 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



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
  - Seach 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)