



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



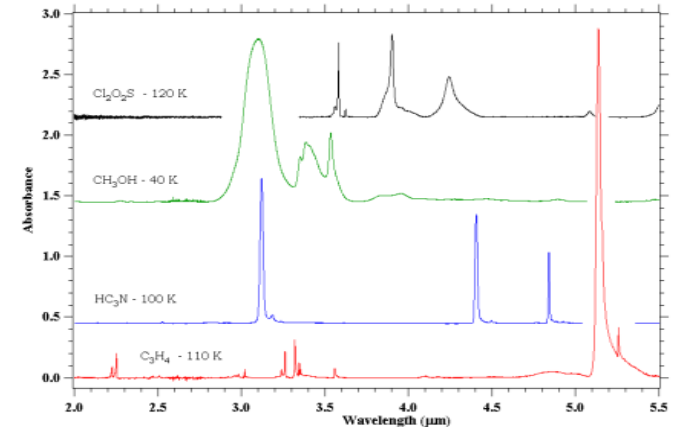
Main aim of *SSHADE*

- **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* ?

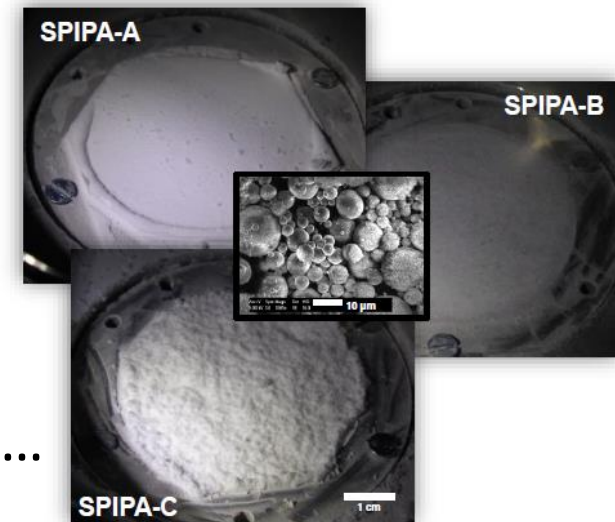
• Materials

- **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 γ -rays to radio wavelengths
- Now mostly **from near-UV to sub-mm (0.3 μ m - 1mm)**, plus **X-rays**.

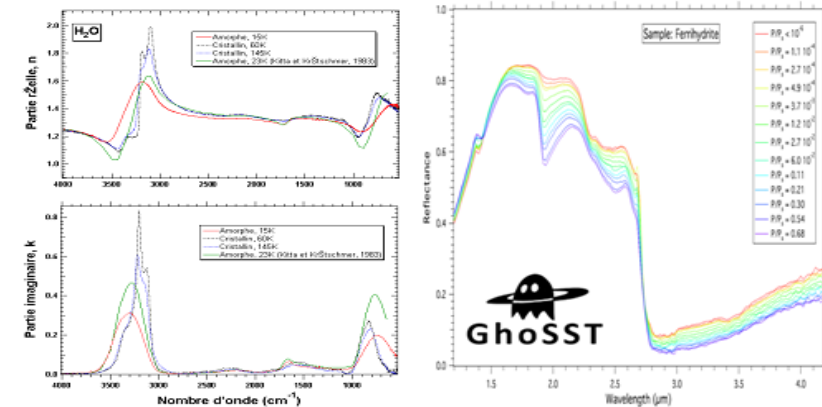
- **Types of data:**

- **Spectra**

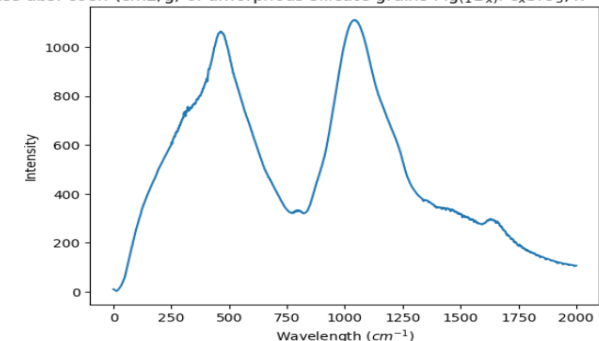
- **Transmission** spectra, absorption coefficients, **optical constants** ...
- **Reflectance** spectra of surfaces, spectro-photometric functions, ...
- **Raman** spectra & micro-spectroscopy, *Fluorescence*, ...
- **XANES** spectra

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

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



Mass abs. coef. (cm²/g) of amorphous silicate grains Mg_(1-x)Fe_xSiO₃, x=0.3



SSHADÉ European Consortium of Data Providers

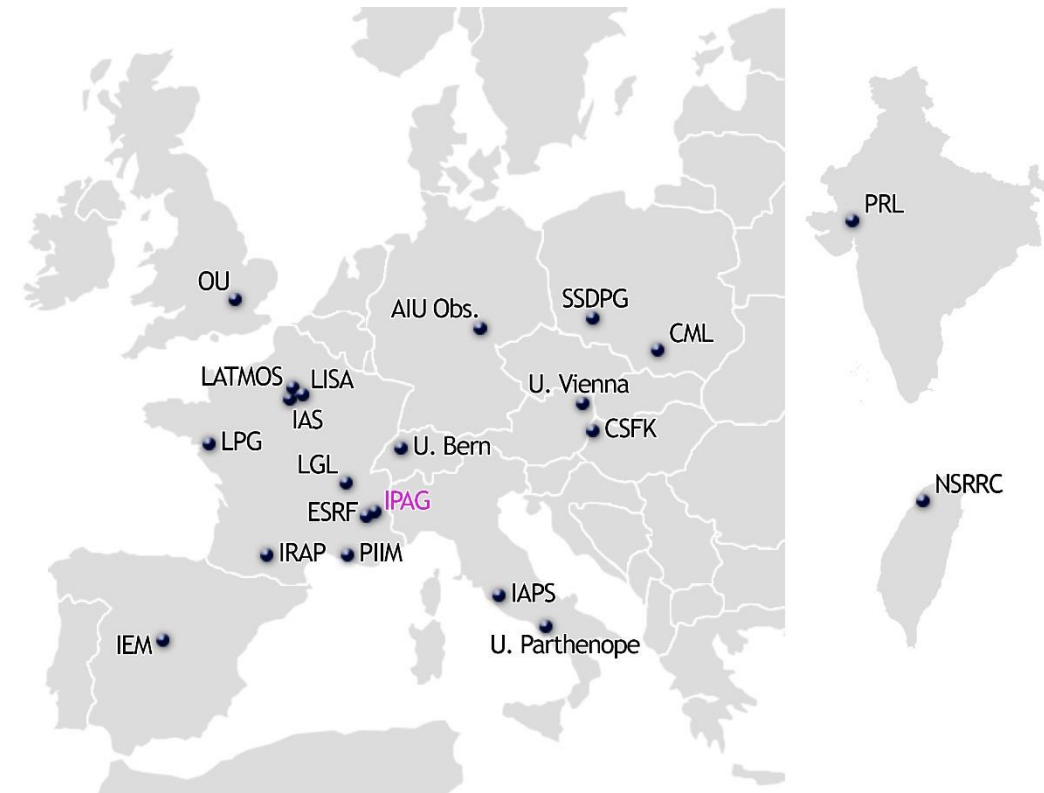
Data from **23** solid spectroscopy experimental groups
in **8** European countries (F, PL, D, GB, CH, E, I, HU) +India +Taiwan
~**75** researchers

Each with particular expertise on:

- some wavelength ranges
- specific techniques
- type of materials and phys.-chem. conditions
- type of data and products, ...

13 active databases + 4 starting + 2 coming

List on SSHADÉ Wiki : <https://wiki.sshade.eu>



SSHADe Web interface

SSHADe online **1st February 2018** at:

<https://www.sshade.eu>

Already in SSHADe:

~ 1400 spectra from > 1000 samples

SSHADe Web interface

Search

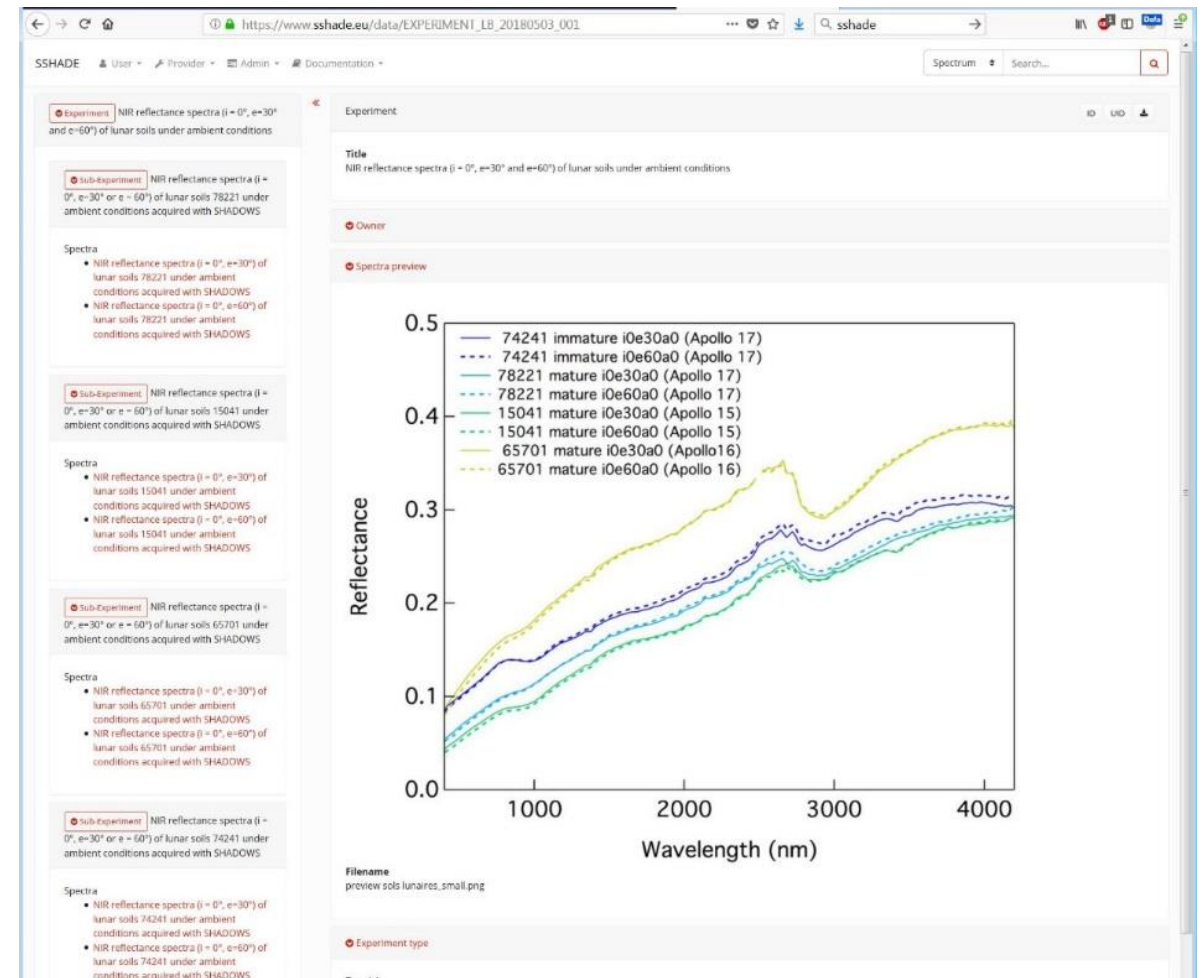
- ✓ Spectra
- ✓ Publications
- ✓ Bandlist

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

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 SSHAE Web interface search results page. At the top, there is a navigation bar with "SSHAE" and user options: "User", "Provider", and "Admin". Below this is a "Spectra search" header. A search input field contains the keyword "meteorite". To the right of the input field are options for "in all fields", "Filters", and a "Search" button. Below the search bar, it indicates "Results: 229 spectra". The main content area displays a list of search results, each with a title and a set of action icons (unfold, quick view, download). The results include:

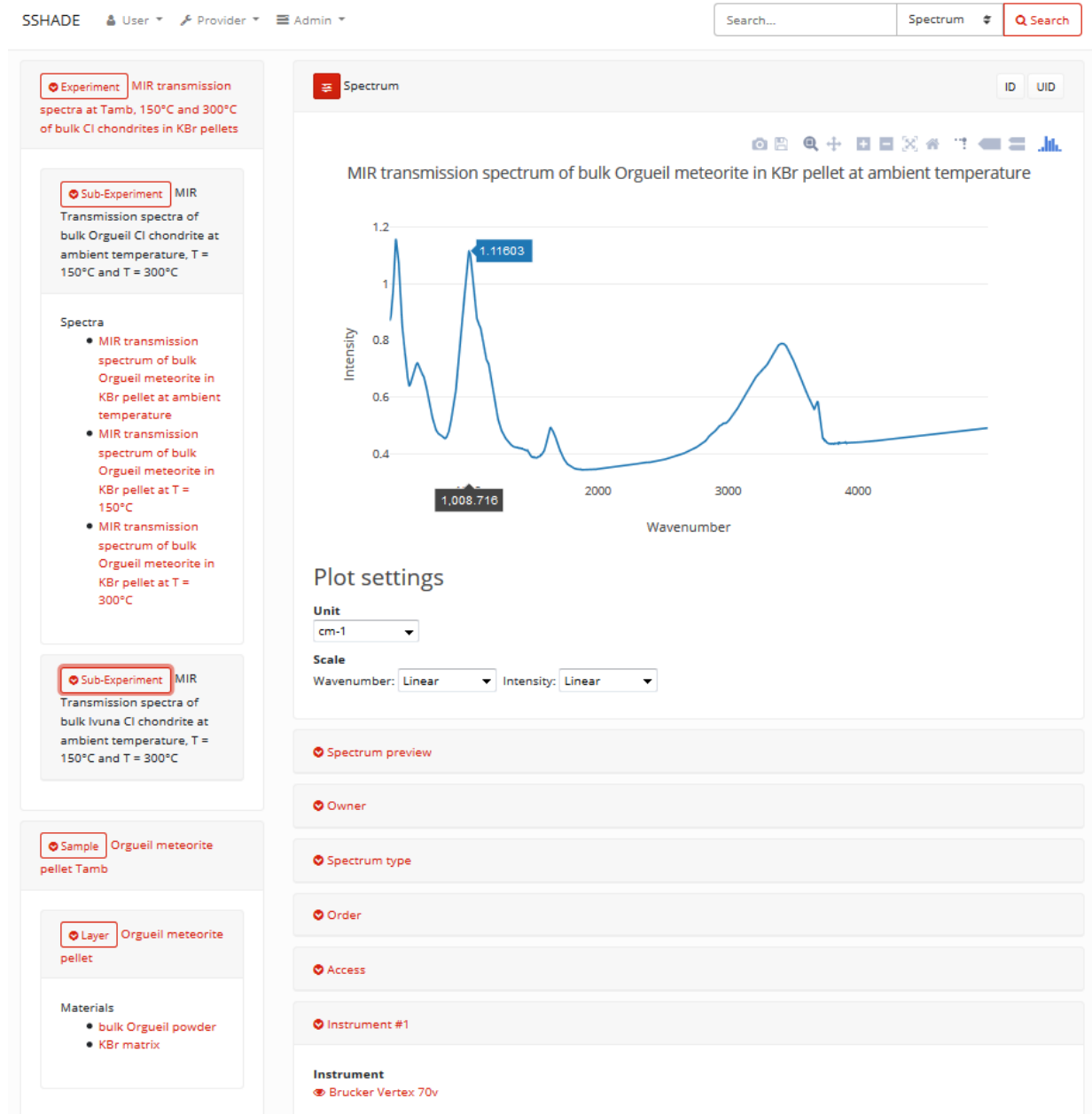
- Averaged Mid-IR spectrum of irradiated Allende pellet (Ar^+ , fluence $6E15 \text{ ions.cm}^{-2}$)
- MIR transmission spectrum of bulk EET92002 meteorite in KBr pellet at ambient temperature
- MIR transmission spectrum of bulk ALH85002 meteorite in KBr pellet at ambient temperature
- Averaged Raman 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 named 'Orgueil meteorite pellet Tamb'. The interface includes a search bar at the top right and navigation tabs for 'User', 'Provider', and 'Admin'. The main content is divided into two panels. The left panel shows a hierarchical view of the sample structure, including a 'Sample' tab and a 'Layer' tab. The right panel provides detailed information about the sample, including its name, owner, origin, physical characteristics (thickness, diameter, mass, substrate material, and comments), and sample environment parameters (temperature, hydrostatic pressure, and 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

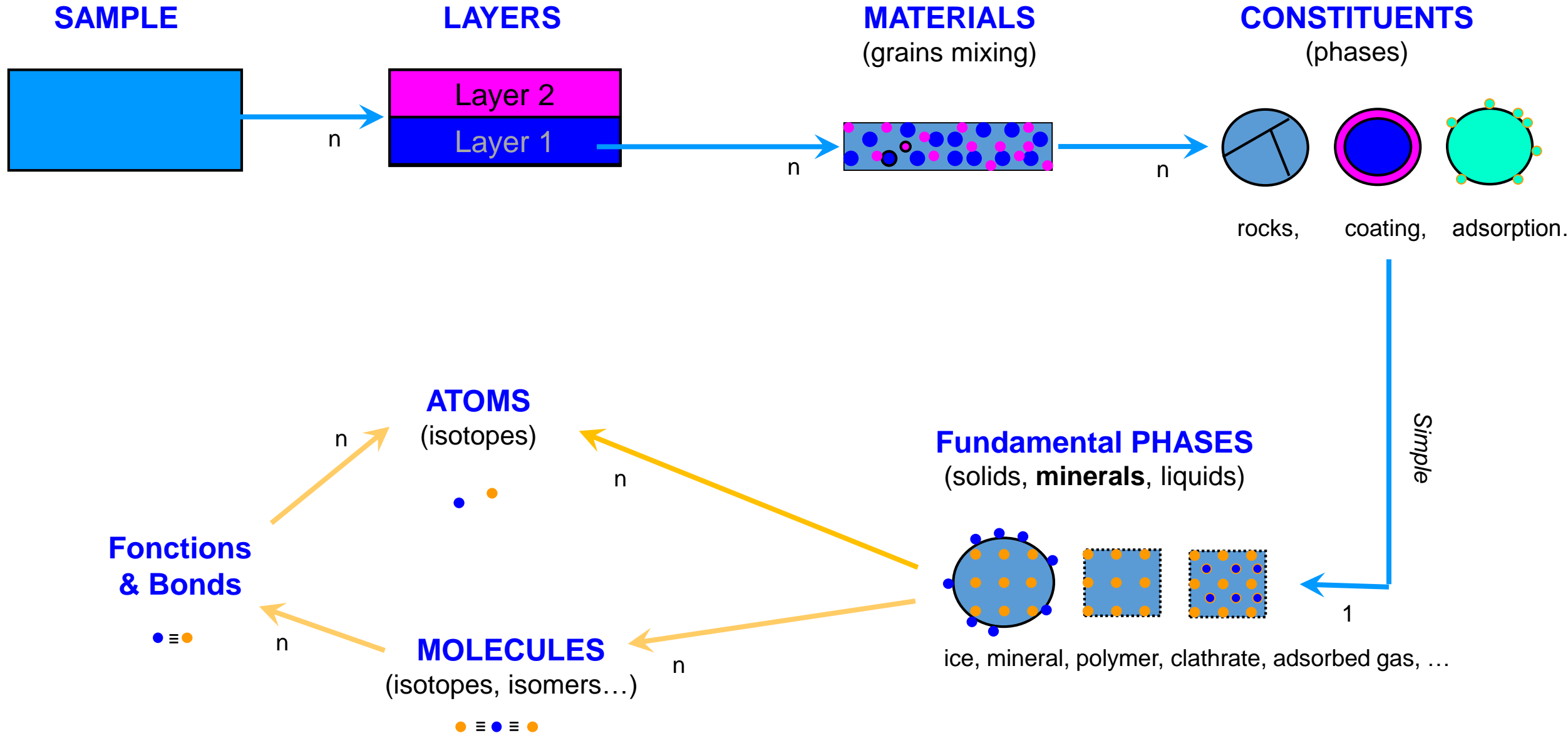
Sample environment: Fluid

Type
vacuum

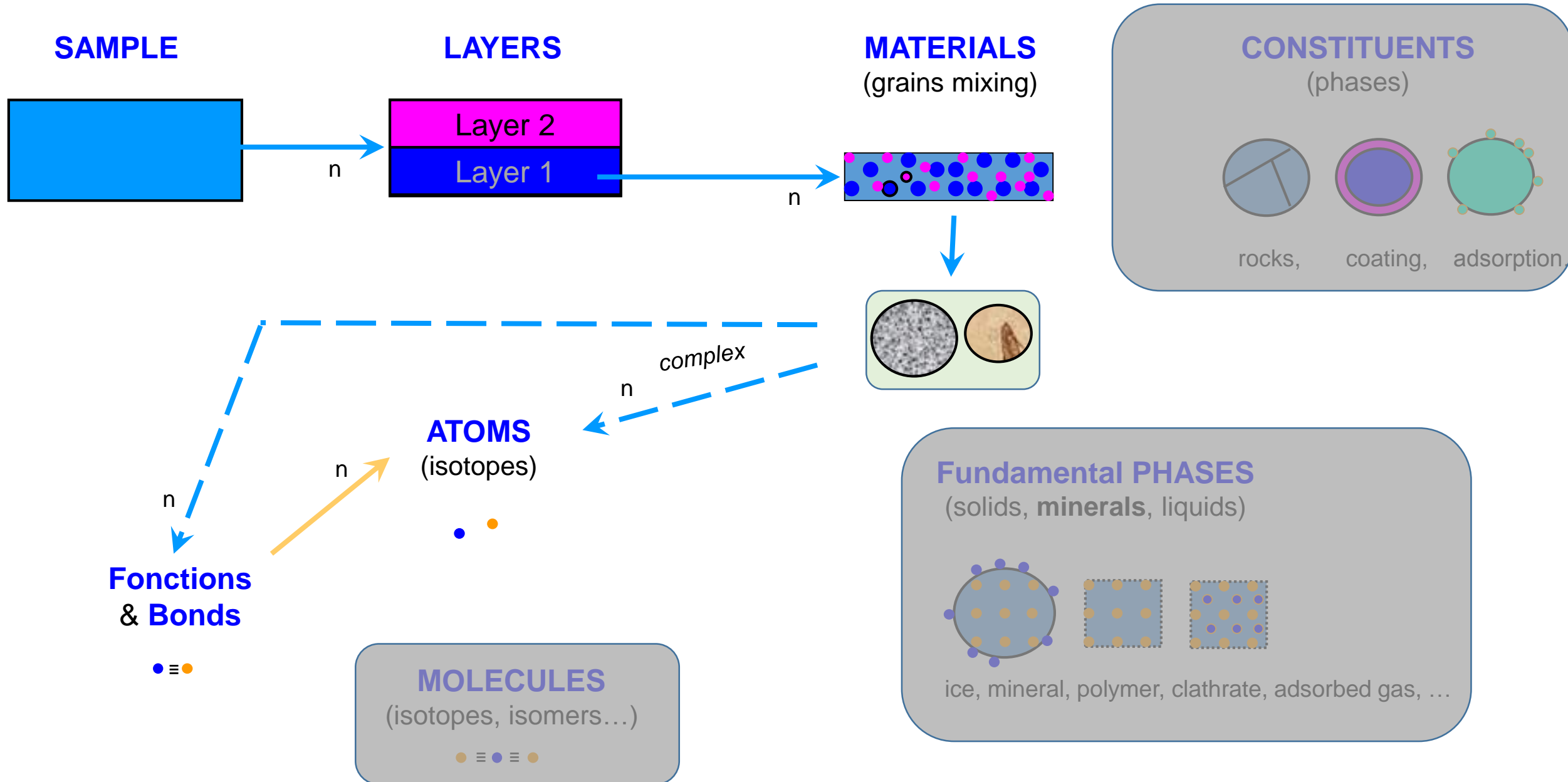
Fluid pressure
0.001 mbar

Comments
stored in a dessicator

SAMPLE description: Layer(s) / Material(s) / Constituent(s)



SAMPLE description: Layer(s) / Material(s) / Constituent(s)



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 content area shows a list of experiments, each with a title and a brief description. A popup window titled 'Related data' is open, displaying detailed information for a specific instrument technique. The popup is divided into sections: 'Instrument technique', 'Instrument description', and 'Technique description'. The 'Instrument technique' section includes the name 'SHINE Spectro-Gonio Radiometer'. The 'Instrument description' section includes the type 'spectro-gonio radiometer', the name 'SHINE Spectro-Gonio bidirectional reflection Vis-NIR', the technique 'bidirectional reflection', and comments 'with series of 6 high pass filters to eliminate high diffraction orders'. The 'Technique description' section includes the technique type 'macroscopic', the source 'Tungsten/Halogen lamp', the source wavelength 'Vis-NIR', the source power '250 W', the spectral analyzer(s) 'diffraction grating 1200 l/mm - 250nm, diffraction grating 600 l/mm - 400nm, diffraction grating 300 l/mm - 1000nm', and the detector(s) 'Si, InSb (cryocooler)'. The background shows a list of experiments with titles like 'NIR bidirectional reflection spectra (i=0°/e=30°) of Smectite SWy-2 with 1.44% adsorbed-interlayer H2O at -30°C'.

SSHAE Web interface

Export

Can export:

- Spectra
- Experiment (several of its spectra fit)

At different level of the interface

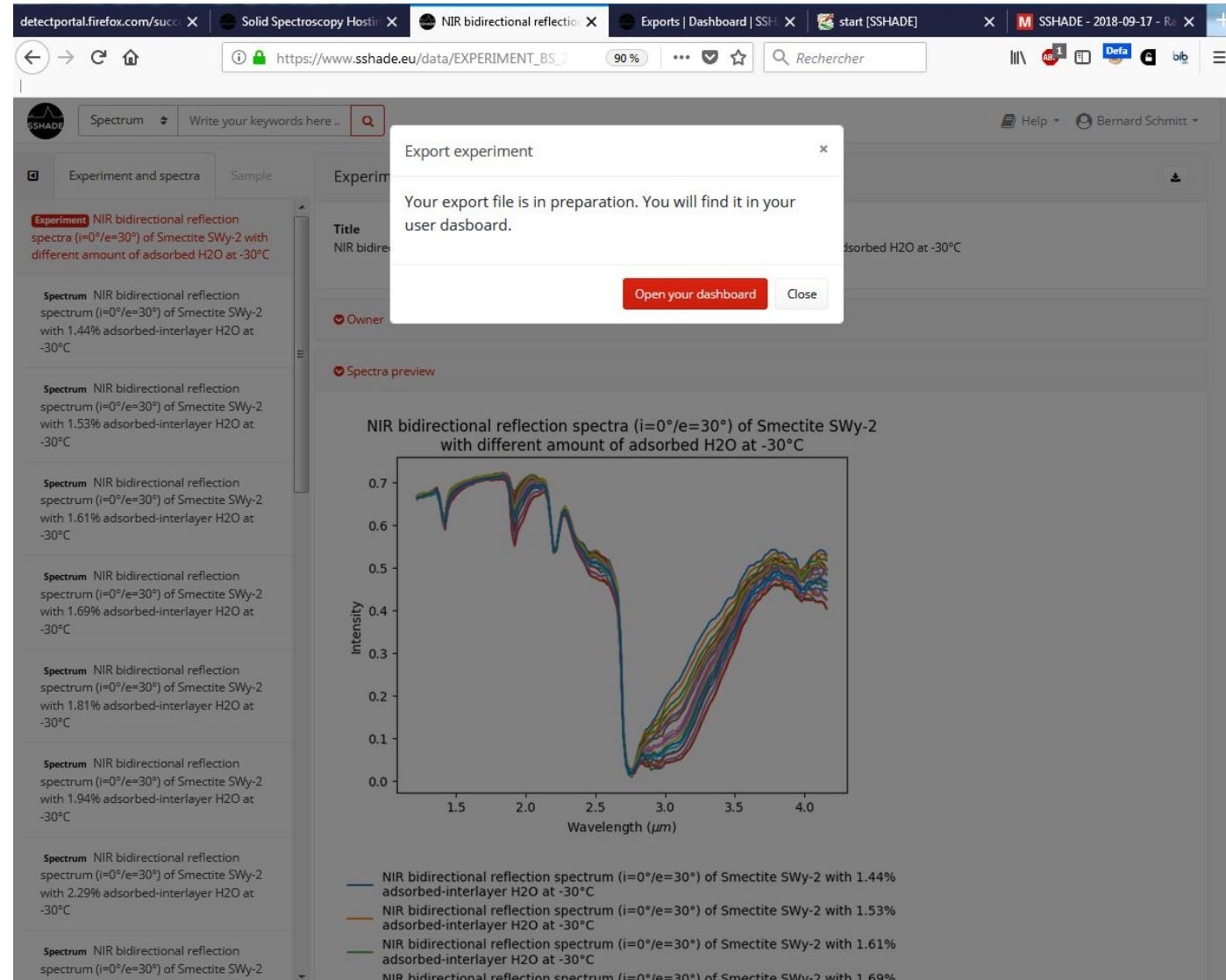
- Search results
- Detail pages of experiment and spectra

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



SSHADÉ 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 'Exports' section of the SSHADÉ user dashboard. On the left is a navigation menu with 'Exports' highlighted. The main area contains a table of export records.

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>done</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>done</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>done</div></div>	0s

User profile

Your informations

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

The screenshot shows the 'Identity' section of the SSHADÉ user profile. On the left is a navigation menu with 'Identity' highlighted. The main area displays personal information and a list of laboratories.

Identity Change password Edit

E-Mail
Bernard.P.Schmitt@gmail.com

First name
Bernard

Family name
Schmitt

ORCID
0000-0002-1230-6627

Laboratories Add

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 Wiki

SSHADE infos

SSHADE fact sheet
List of databases

User help (interface documentation)

Interface guide

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

Data search guide

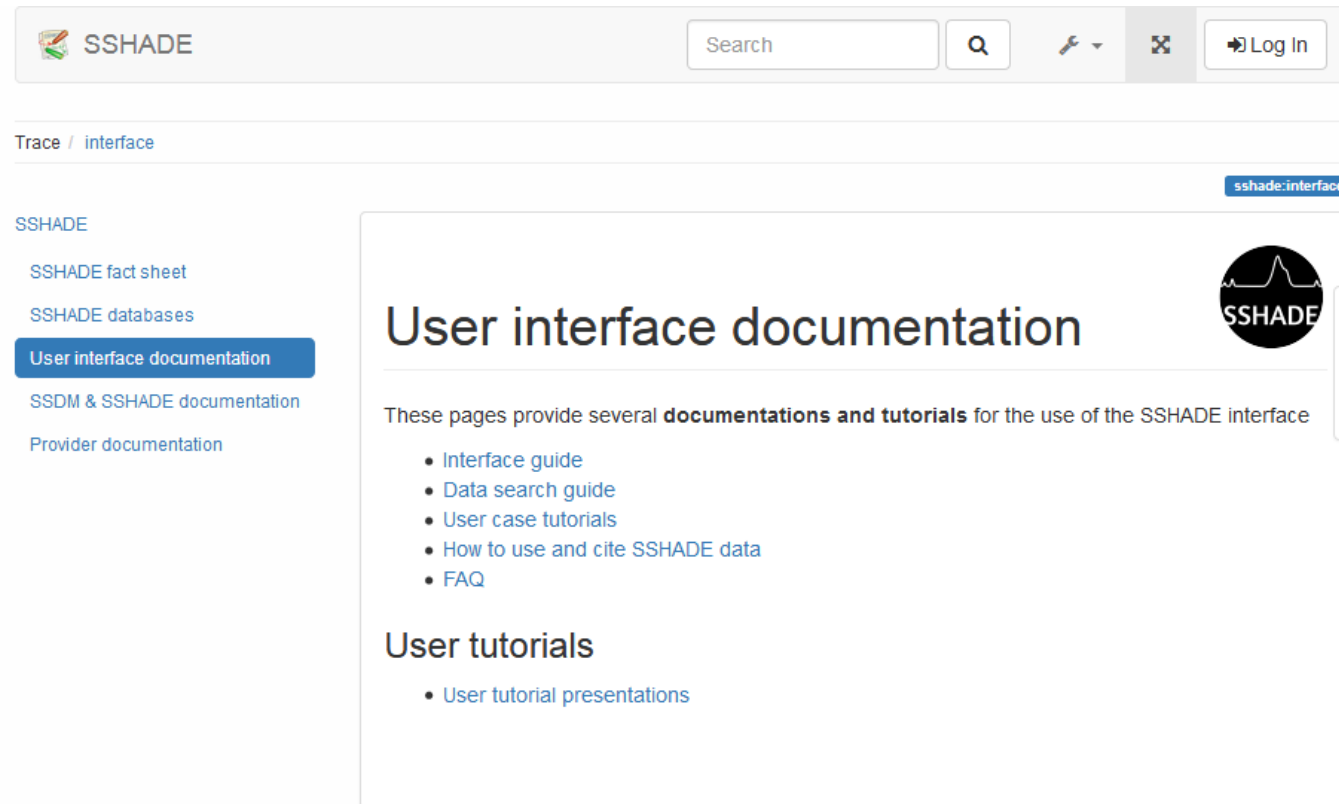
- Google-like search bar
- Filter search tool

User tutorials

Future developments

- User cases videos

<https://wiki.sshade.eu>



The screenshot shows the SSHADE Wiki user interface documentation page. At the top, there is a navigation bar with the SSHADE logo, a search box, and a 'Log In' button. Below the navigation bar, the page title is 'Trace / interface'. The main content area is titled 'User interface documentation' and contains a list of links to various documentation and tutorial pages. The left sidebar lists the following items: SSHADE, SSHADE fact sheet, SSHADE databases, User interface documentation (highlighted), SSDM & SSHADE documentation, and Provider documentation. The main content area lists the following items: Interface guide, Data search guide, User case tutorials, How to use and cite SSHADE data, FAQ, User tutorials, and User tutorial presentations.

SSHADE

Search

Log In

Trace / interface

SSHADE

SSHADE fact sheet

SSHADE databases

User interface documentation

SSDM & SSHADE documentation

Provider documentation

ssshade:interface

User interface documentation

These pages provide several **documentations and tutorials** for the use of the SSHADE interface

- Interface guide
- Data search guide
- User case tutorials
- How to use and cite SSHADE data
- FAQ

User tutorials

- User tutorial presentations

SSHADDE on-line DEMO

www.sshade.eu

Scenario SSHADE demo (1):

- **Home page**
 - Search bar (all databases)
 - List of active/starting databases
 - Search filtered by database
 - Details on each database
 - Search bar
 - 2 possibilities: spectra & Publications
 - Search 'Google-like' (english): « Moon »
- **Page search results**
 - Top Menu (see later)
 - Search bar + filter (later 2nd ex)
 - Number of results
 - 2 results: 1exp w. 4 soils/8 spectra, 1 spectra meteorite
 - Structure of results: exp + spectra
 - Concept of experiment
 - ✓ Sample w variable param (1 to 3)
 - ✓ Sample evolving (irrad., ads., ...)
 - ✓ Set of similar samples
 - ✓ Any combination
 - Preview, export
 - View

Scenario SSHADE demo (suite - 2):

- **Visu « meteorite MIR transmission Allende »**
 - Structure page
 - Left: tabs experiment + sample (fold)
 - Right: details page
 - Left: tabs experiment / spectra
 - push left
 - Structure 'sub-exp' / spectra
 - un/fold
 - Right: Page experiment
 - Publi ?
 - Instrument
 - ...
- **Page spectrum + sample preview**
 - Static spectrum preview
 - Publi + links
 - Main info on spectrum + sample
 - Links to sample
 - Direct download
 - Eye: spectrum details

Scenario SSHADE demo (suite - 3):

* Page Interactif spectrum + details

- Spectrum plot (valid range)
 - ✓ Zoom, position, ...
 - ✓ Change of units, log axis
 - ✓ download png
- Spectrum details
 - Range, resolution ...
 - Sample link (but also left tab)

* Left tab: sample structure

- Overview structure layer/Mat./Const.
 - un/fold
- Allow to directly see details at all levels

➤ Right page: sample details

* Page Sample details:

- image, T, P, publi

* Page Layer details:

- Thickness, ...

* Page Matter details:

- Materials
- object

* Page Constituent

- species

Scenario SSHADE demo (suite - 4):

* Search « Lunar soil » or « apollo »

- 2 results: 4 soils/8 spectra,
 - Download exp (all spectra)

* Left: Visu Exp:

- structure Exp in 4 subexp (4 soils)
- 2 spectra per sub/exp
- Active spectrum
- Corresponding samples

* Filter search

- ✓ work with search bar
- Search bar 'Meteorite' + 'CM'
- Search filters
 - by experiment,
 - by instrument parameters,
 - by environment,
 - by extra-terrestrial object,
- Search filter 'CO', 'CM'
 - by extra-terrestrial object
 - Class ? (marche pas)

Scenario SSHADE demo (suite - 5):

* Filter search

- ✓ Useful
 - ✓ when you have too much results
 - ✓ for numerical values constraints (T, P,diam)
 - ✓ when KW with possible confusion
 - ✓ When you don't know what word to use
- ✓ 3 types of keywords
 - ✓ Free: type word
 - ✓ Sart, contain, ...
 - ✓ wildcard
 - ✓ Enum:
 - ✓ choice one or more
 - ✓ Select all / unselect
 - ✓ Numerical
 - ✓ Values or range
 - ✓ =, >, <, ...

* Search Smectite

- Search 'smectite +NIR'
- Search filter:
 - by instrument parameters
 - Enum: Select several [sample origin]
 - 'diff type reflectance'

Scenario SSHADE demo (suite – 6)

- Search filter
 - by sample,
 - Temperatue: 240-260
- Reset
 - KW
 - Bar
 - filters

Scenario SSHADE demo (suite - 7):

➤ **Export**

- Experiment (smectite temperature)
 - Dashboard
 - List of spectra
 - Download zip file
 - Open zip file
 - Content
 - Description file
 - Data file (ascii)
 - Metadata
 - HTML file with Internal links
 - Exp/spectra
 - Sample/layer/Mat./Const.
 - Experiment
 - Spectra
 - Associated sample
 - Citations file
 - Publications
 - DOI (soon)
 - Link to original experiment (UID)

Scenario SSHADE demo (suite – 8)

* **Publication search**

- Search bar
- Filters
 - by reference
 - Authors
 - Journal
 - Doi...
 - by content
 - by published spectrum

• **User account**

- Menu 'user'
 - Complete your profile
 - Add your lab
 - Future
 - Store search preference

* **Wiki**

- Menu: 'Help': 'wiki' or 'user guide'
 - List databases
 - Interface doc
 - provider area (restricted)