



*Journées ASOV  
Paris – 10 March 2020*

## L'infrastructure de données SSHADE de spectroscopie des solides: état des lieux de son développement et évolutions futures



<https://www.sshade.eu>

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



# The SSHADe database infrastructure

for Astrophysics, Planetary sciences and Geosciences

**Promote** the creation of databases and **develop** the tools to provide on-line experimental data on **spectra of solids** in the **electromagnetic spectrum**

→ Set of databases from a Consortium of laboratories



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

# SSHADE European Consortium of Data Providers

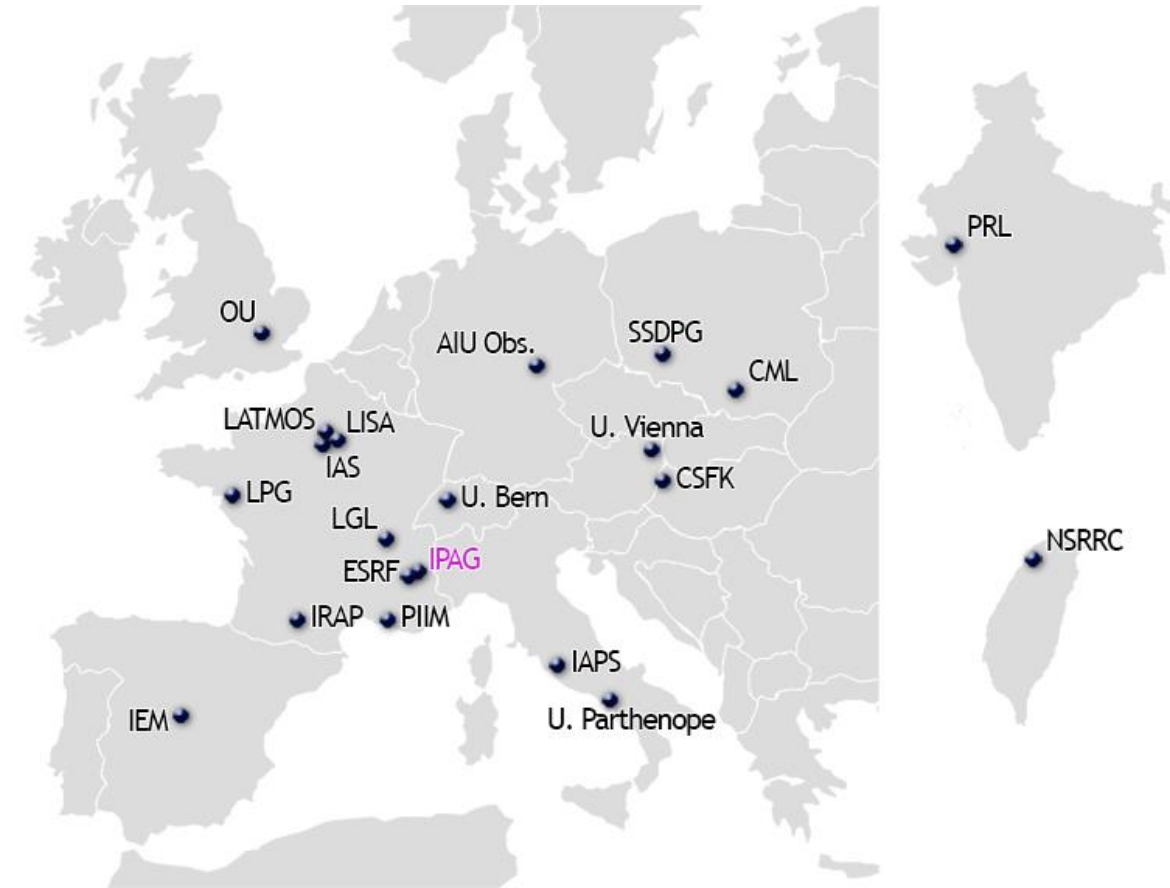
Data from **23** solid spectroscopy experimental groups  
in **8** European countries (F, PL, D, GB, CH, E, I, HU) + India + Taiwan  
~**75** researchers

## Each with particular expertise on:

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

**17 active databases + 2 starting**

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



# A little bit of history: from past to future

- 2002-2006: Idea ... Concept ... Content demonstrator: STSP
- 2007-2008: First “solid spectroscopy” datamodel, Dev. technical demonstrator (OSUG, ...)
- ✓ **2009-2012:** **Full developments (Europlanet + VAMDC – FP7) of:  
SSDM (Solid Spectroscopy Data Model) and GhoSST database infrastructure**
- July 2011 GhoSST functional prototype
- ✓ **25 Sept. 2012:** **GhoSST opened to the public (v0.5 beta-version )**
- 2013-2015: Continuing SSDM and GhoSST developments, GhoSST data feeding
- 2014 Preparation and opening of a pre-SSHADE database
  
- ✓ **2015-2019:** **Development of SSHADE infrastructure under EPN@2020-RI (VESPA JRA)  
Opening of SSHADE to participating European (+Indian) partners (VESPA VA)**
- ✓ **1 Feb. 2018:** **SSHADE online with 10 databases (1250 spectra)**
- Feb. 2020: SSHADE with 17 active databases (> 2700 spectra)
  
- ✓ **2020-2023** **Europlanet-2024 RI : development of ‘band list’ database  
Addition of 10-12 databases from around the world**

# **Solid Spectroscopy Data Model**

**Recent SSDM Changes / Improvements**

# Major upgrade of SSDM (v 0.9.0)

- **Databases:**
  - added KW to fully manage your database entry page @ SSHADE
  - added options to complete DOI information
- **Molecules:**
  - better and simpler description of 'stereo-isomers' and 'nuclear spin' isomers
- **Phases:**
  - better description of crystal sites (atoms, molecules), and polymers
- **Bodies:**
  - **new table describing planetary bodies** w. some physical parameters (linked from Objects)
- **Objects:**
  - new 'planetary objects' (**samples collected on planetary bodies**) [to be completed]
  - possibility of geolocation of objects (planetary or extraterrestrial\*)
- **Matters:**
  - some extensions for planetary matters (sample return)
  - possibility of **geolocation of matters** (planetary, including Earth)
- **Sample:**
  - added matter/material grain size median + width. Added crystals (sizes, ...) in Constituent, ...
- **Publications:**
  - added other publication identifiers type and code (ex: ArXiv, ...) + free URL

# Major upgrade of SSDM (v 0.9.0)

- **Experiment & matters**

- added **DOI support** (completed)
- Inclusion of field and airborne measurements
- Addition of geolocation of natural samples (collected or field measurement)

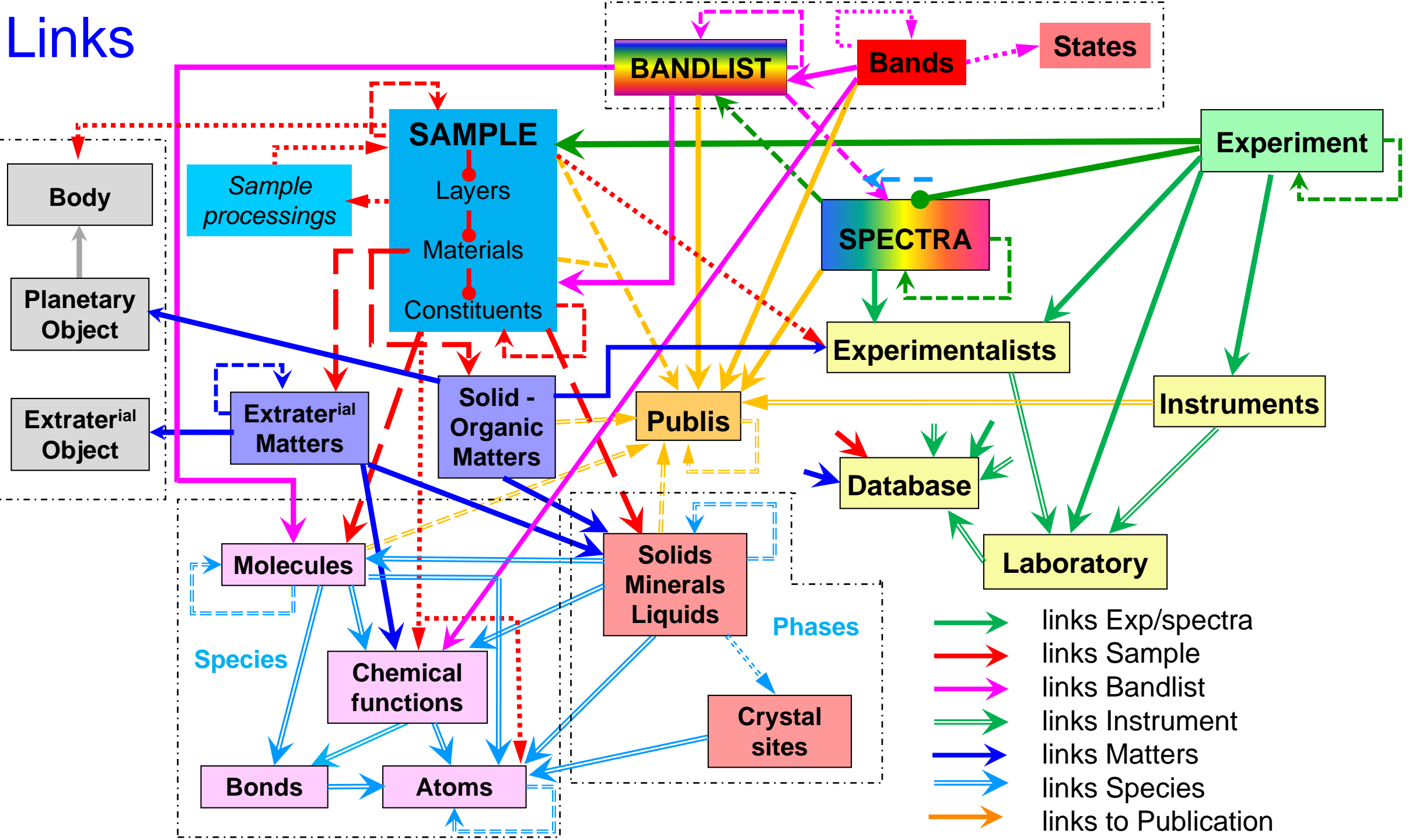
- **Spectra:**

- Better description and import of **multi-angle data** (BRDF, ...)
- Improvement of experiment/spectra **version management** (to be finalized)
- Addition of several preview options for experiment and spectra
- **Extension** of the spectral range and spectrum types **to radio wavelength**
- Extension to Polarized spectra (specific import format to be finalized)
- Extension to Scattering measurements
- Extension to reflectance model parameters: (but not yet specific import format for set of n parameters)

- **Everywhere:**

- removed some unnecessary mandatory or improved conditions
- extended several Enum/OpenEnum with your suggestions
- extended size of some text KW
- improved description & comments in xml and SSDM, ... ..

# Links

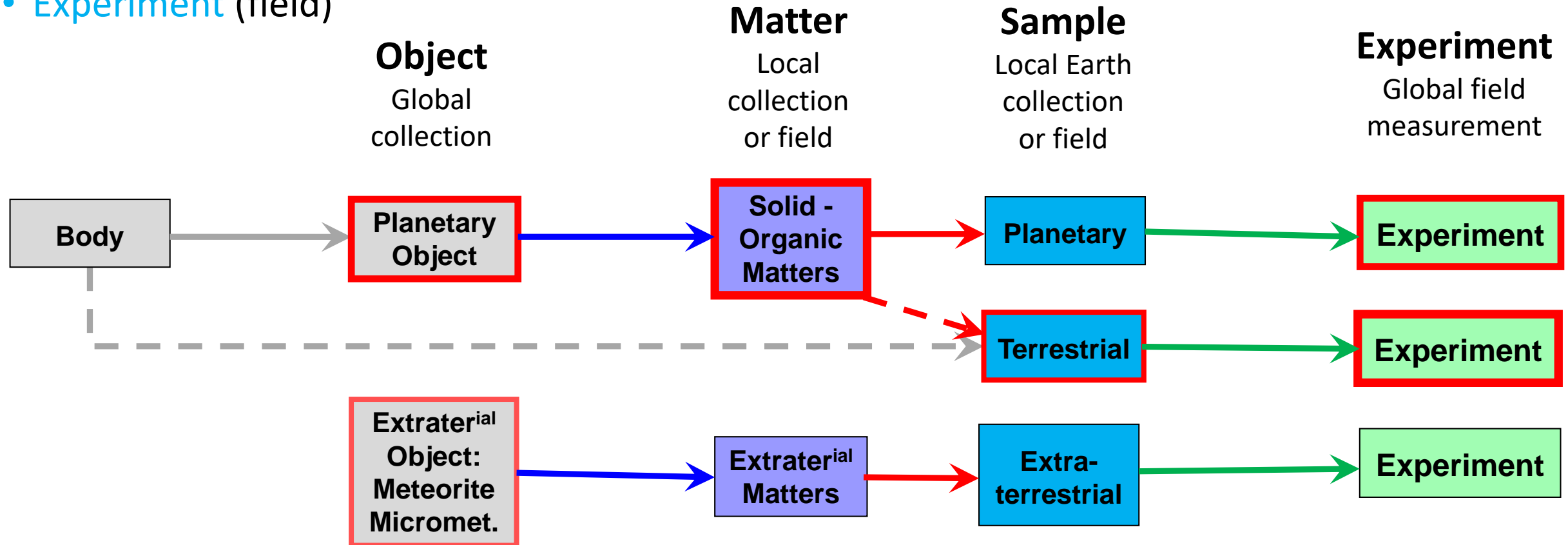




# Geolocation: collection and field measurements (v 0.9.0)

- **Objects** (except IDPs)
- **Matters** (except extraterrestrial)
- **Sample** (simplified case for Earth)
- **Experiment** (field)

- Body or object, Place, country
- Coordinates
  - System, type
  - Lat/long, altitude



# Description and import of multi-angle spectral data (v 0.9.0)

- **Surface spectra with 3D angles (illumination – observation – azimuth) :**

- « spectrum\_type »: physical measurement type
- « spectral\_observation\_mode » : spectrum, multi-wavelength, ...
- « angle\_observation\_geometry »: direct, bidirectional, directional-hemispheric, ...

## 4 import options depending on dataset organization in original file(s):

- unique file with full spectro-photometric data set
- series of spectrum files at single geometry in a multi-angle dataset
- series of photometric data files at single wavelength in a multispectral dataset
- series of spectro-photometric data files with a single data type in each file

**→ all data homogeneously stored in the same 4D structure  
with same angle definition !**

+ read and import the 3 specific formats from Bern, IPAG and IRAP

+ selection of spectra within spectro-photometric data for experiment preview

# Better versions management (v 0.9.0)

- **Spectrum versions:**

- 2 options

- New version:

- Explanation what is new
    - Import new spectrum
    - Keep old version(s) with metadata

- Invalidate:

- Explanation why it is invalidated
    - Keep invalidated version(s) with metadata
    - Possible link to another spectrum with equivalent data

- **Experiment versions:**

Detemined from spectrum version

- New version:

=> new experiment DOI (extension .Vn) **(TBD)**

➔ **INTERFACE:**

- Tell if obsolete/invalidated and when a new version exists
- Provide version & correction history

The screenshot displays the SHADP web interface. At the top, there is a search bar with the text 'Spectrum' and a search icon. Below the search bar, the interface is divided into two main panels. The left panel, titled 'Experiment and spectra', shows a tree view of the data structure. It includes a 'Sample' section with a 'Sub-Experiment' for 'sample thickness' containing three 'Full spectrum' entries. Below this, there are two 'Sub-Experiment' sections for 'emergence angle 1' and 'emergence angle 2', each containing three 'Full spectrum' entries. The right panel, titled 'Spectrum history', displays a table of version changes. The table has columns for Date, Mode, Version, Status, and Comments. The history shows several entries, including obsolete versions, corrections, and new versions, with some versions being partially invalidated.

Date	Mode	Version	Status	Comments
2019-05-14 16:55:19 UTC+0000	first import	#1	obsolete version	2007-00-00: new bidirectional reflectance spectrum (NIR) of 5.16% H2O adsorbed on Palagonite
2019-05-14 17:19:40 UTC+0000	correction	#1	obsolete version	2007-00-00: new bidirectional reflectance spectrum (NIR) of 5.16% H2O adsorbed on Palagonite
2019-05-19 06:43:11 UTC+0000	correction	#1	obsolete version	2007-00-00: new bidirectional reflectance spectrum (NIR) of 5.16% H2O adsorbed on Palagonite
2019-05-20 17:28:41 UTC+0000	new version	#2	partly invalidated version	import new version
2019-05-27 17:01:58 UTC+0000	new version	#3	partly invalidated version	import new version
2019-05-27 17:20:08 UTC+0000	correction	#3	partly invalidated version	import new version
2019-05-27 17:37:02 UTC+0000	new version	#4	valid version	import new version
2019-05-29 16:17:58 UTC+0000	correction	#4	valid version	2007-00-00: new bidirectional reflectance spectrum (NIR) of 5.16% H2O adsorbed on Palagonite
2019-05-29 16:34:12 UTC+0000	correction	#4	valid version	2007-00-00: new bidirectional reflectance spectrum (NIR) of 5.16% H2O adsorbed on Palagonite
2019-05-29 16:38:32 UTC+0000	correction	#4	valid version	2007-00-00: new bidirectional reflectance spectrum (NIR) of 5.16% H2O adsorbed on Palagonite

# SSDM – future evolutions (2020...)

- Future options to be developed ( $\geq 2020$ )

- **Bandlists** (upgrade from GhoSST) + **band parameters**

[Europlanet-2024 RI]

- Implementation of 4-parameters **polarization** import and storage

[2020 ?, when import/storage formats fully defined]

- Implementation of n-entries **model parameters** import and storage

(when ?)

- Implementation of **spectro-images** import and storage

(later ...?)

- Addition of several **fundamental physical properties** of solids (Ps, thermodynamic properties, ...)

(2021/22...?)

# Development of SSHADE interface

# Development of SSHADE interface

## A lot of new features and tools !!!

- For users: Login / Search / Visualization / Export / Dashboard
- For data providers: Detailed search, import, verification/publication tool
- For SSHADE managers: management of database, providers, members, ....

Better organized, More efficient, More stable, ....

# User: Search interface

- **Search tool:**

- ✓ more efficient top search bar based on « **Elasticsearch** »
- ✓ more filters choice
- ✓ Reset modes: global, per keyword
- ✓ ...

- **Result list :**

- ✓ Well working experiment grouping

The screenshot displays the SHADE search interface. At the top, there is a search bar containing the text "Moon, Apollo" and a search button. Below the search bar, there are several filter categories, each with a "Reset" button. The categories are:

- By experiment**
- By instrument parameters**
  - Technique: in (Nothing selected)
  - Spectral
    - Observation mode: in (multi wavelengths, spectrum)
    - Spectral range type: in (Nothing selected)
    - X absorption edge element: is
    - X absorption edge type: in (Nothing selected)
  - Polarization
    - Illumination polarization type: in (Nothing selected)
    - Observation polarization type: in (Nothing selected)
  - Angular
    - Observation geometry: in (bidirectional, conical-hemispheric, directional-hemispheric)
  - Spatial
    - Macro-, microscopy, imaging: in (microscopy)
- By environment**
- By extraterrestrial object**
- By sample**
- By composition**

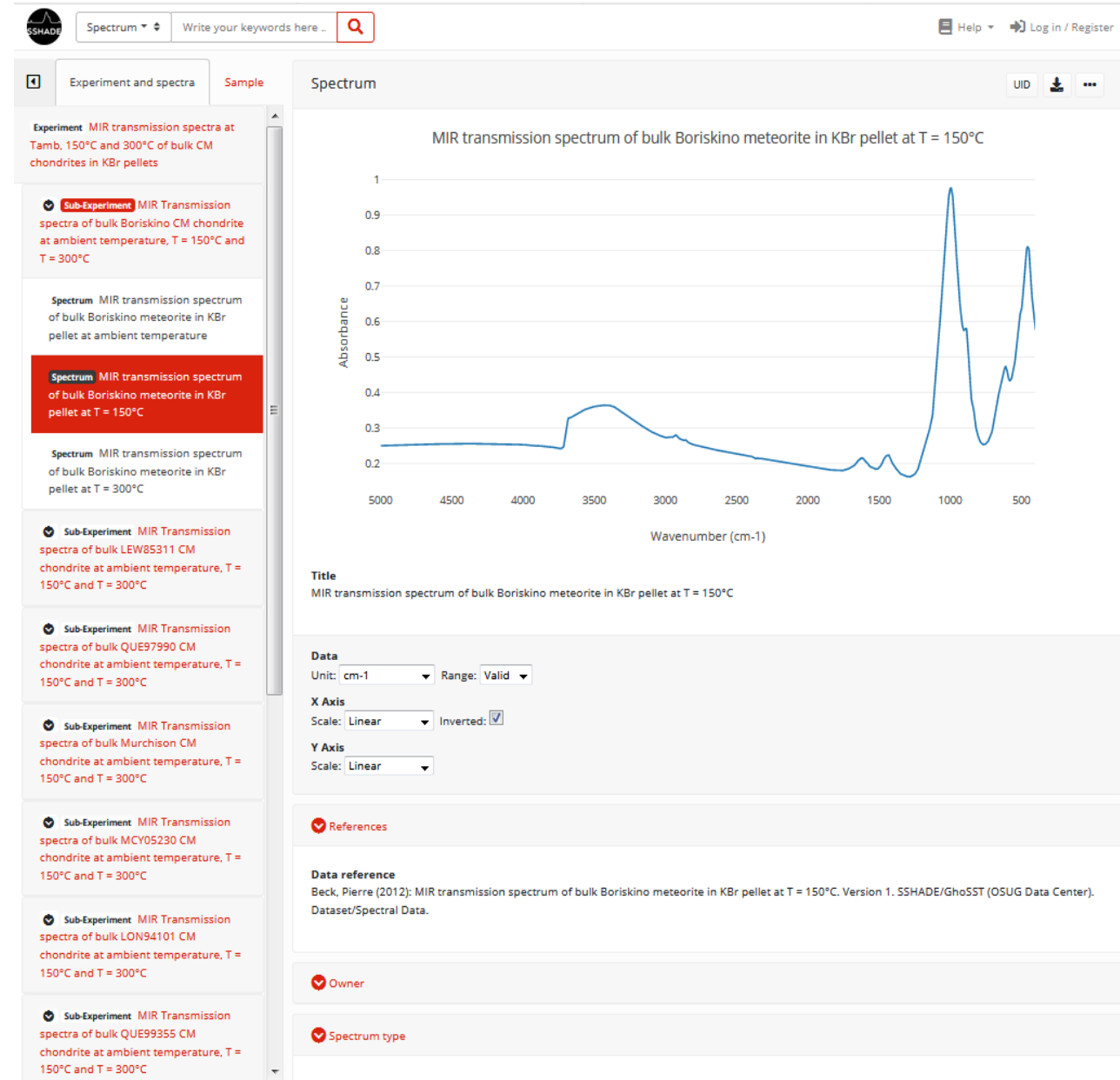
A dropdown menu is open under the "Spatial" filter, showing a list of options: "macroscopic", "microscopy" (highlighted in red with a checkmark), "linear scan", "linear micro-scan", "imaging", and "micro-imaging". The dropdown also includes "Select All" and "Deselect All" buttons.

# User: Experiment-spectra / Sample data interface

- **Experiment display :**

## Better structuration

- ✓ Exp-spectra and sample Tabs
- ✓ Highlight of displayed data
- ✓ Highlight of spectra with common sample
- ✓ ...





# User: Experiment-spectra / Sample data interface

- **Experiment display :**

## Better structuration

- ✓ Exp-spectra and sample Tabs
- ✓ Highlight of displayed data
- ✓ Highlight of spectra with common sample
- ✓ ...

- **Samples :**

- ✓ Highlight of displayed sample structure level
- ✓ Collapside structure still TBD

The screenshot displays the SSHADE web interface. At the top, there is a search bar with the text 'Spectrum' and 'Write your keywords here'. Below the search bar, there are two tabs: 'Experiment and spectra' and 'Sample'. The 'Sample' tab is active, showing the following information:

- Sample:** Boriskino meteorite pellet T150
- Layer:** Boriskino meteorite pellet heated at 150C
- Material:** pellet of bulk Boriskino and KBr heated at 150C
- Constituent:** matrix Boriskino heated at 150C (highlighted in red)
- Constituent:** chondrules Boriskino IPAG
- Constituent:** CAIs Boriskino IPAG
- Constituent:** adsorbed water on Boriskino bulk
- Material:** KBr matrix
- Constituent:** KBr
- Constituent:** adsorbed water on KBr (Beck14)

On the right side, there is a 'Constituent' panel with the following details:

- Name:** matrix Boriskino heated at 150C
- Type:** (checked)
- Family:** complex mix
- Class:** mixed molecular solid
- Compound type:** complex organic-mineral mix
- Comments:** 38.4 vol% of matrix in Boriskino meteorite (Alexander et al., 2007) - matrix = mixture of minerals and organics - Matrix heated at 150°C for 2h => possible composition and state evolutions

Below the constituent details, there are three sections with expandable options:

- Constituent abundance in material (checked)
- Chemical composition (checked)
- Species (checked)

The 'Species' section is expanded, showing a table of chemical species:

	Formula	Name	Family	Number min-max	Mole fraction	Mass fraction	State	Relevance	Comments
⊕	C	Carbon	element			0.18 ± 0.01	in complex	main	0.18 wt% of C in the matrix, unknown abundance of other atoms - data from Alexander et al. (2007)
⊕	H	Hydrogen	element				in complex	main	
⊕	O	Oxygen	element				in complex	main	
⊕	N	Nitrogen	element				in complex	main	
⊕	Si	Silicon	element				in complex	main	

# User: Dashboard interface

- **Dashboard:**

- ✓ Export history (date, export progression, download, link for sharing, view, ...)
- ✓ Import history (date, source file, download)

The screenshot displays a user dashboard with a sidebar on the left and a main content area on the right. The sidebar includes navigation links for Dashboard, Exports, Imports, Searches, Profile, Data access, Identity, and Settings. The main content area is divided into three sections: Exports, Imports, and Searches.

**Exports Section:** A table with columns: Export, UID, Title, Export date, Size, Steps, Progression, and ETA. It lists three export entries.

Export	UID	Title	Export date	Size	Steps	Progression	ETA
		EXPERIMENT_AG_20131028_000	2019-06-03		Step 6/9 (Spectrum 5/30)	<div><div style="width: 28%;">28%</div></div>	2m45s
		EXPERIMENT_TEST_KN	2019-05-21	558.2 kB	done	<div><div style="width: 100%;">done</div></div>	0s
		SPECTRUM_FULL_1	2019-05-14	370.8 kB	done	<div><div style="width: 100%;">done</div></div>	0s

**Imports Section:** A table with columns: Date and Source file. It lists five import entries.

Date	Source file
2019-06-01 08:02:49 UTC+0000	63_experiment_spectra_Test- <a href="#">kn_v090.zip</a>
2019-06-01 08:00:16 UTC+0000	63_experiment_spectra_Test- <a href="#">kn_v090.zip</a>
2019-06-01 07:58:26 UTC+0000	64_experiment_spectra_Test- <a href="#">v090_2.zip</a>
2019-06-01 07:56:41 UTC+0000	64_experiment_spectra_Test- <a href="#">v090_2.zip</a>
2019-06-01 07:49:33 UTC+0000	41_matter-solid_Test- <a href="#">v090.xml</a>

**Searches Section:** A section titled "Searches" with a "View all" button and the text "No searches."

# User: Export setting interface

- **Export settings**

- ✓ Unit
- ✓ Spectral range
- ✓ Data and metadata format
- ✓ Export file format
- ✓ ...

Can be set as 'user preferences'  
or at each file export

SSMADE Spectrum Write your keywords here ... Help Bernard Schmitt

User

Dashboard

Exports

Imports

Searches

Profile

Data access

Identity

Settings

Export

Wavenumber / Wavelength / Frequency / Energy

Unit conversion: micron

Number format: Float Decimals: 5

Spectral range

Range type: Whole data range Min: 0 Max: 0

Range unit: micron

Value / Intensity

Number format: Float Decimals: 5

Spectrum data file

Data type: Spectrum data only

File format: CSV

Spectrum metadata file

File format: HTML

Archive file

Archive format: zip

Submit changes Clear preferences

# Data provider: data verification / release interface

- **Unverified Experiments / spectra**

- ✓ Unverified/verified status
- ✓ Verification process

- **Unreleased/Restricted data**

- ✓ Private / Restricted / Public status
- ✓ Publication process
- ✓ DOI generation

- **Public data**

- ✓ DOI upgrade

The screenshot displays the SSMADE data provider interface. At the top, there is a search bar with the text "Spectrum" and "Write your keywords here...". Below the search bar, there are navigation tabs for "Provider", "Manager", and "Admin". The main content area is titled "Provider Unreleased/Restricted spectra" and shows a table of 10 entries. Each entry includes a status icon (eye with checkmark), a status label (Verified, Unreleased, or Restricted), an access label (Unreleased or Restricted), a UID, a title, and an imported date. The table is paginated, showing "Showing 1 to 10 of 12 entries" and navigation buttons for "Previous", "1", "2", and "Next".

Show	Status	Access	UID	Title	Imported
10	Verified	Unreleased	SPECTRUM_FAKE_1	Full spectrum 1 - new version - NIR bidirectional reflection spectrum (i=0°/e=30°/az=0°) of Palagonite JSC Mars-1 with 5.16% adsorbed H2O at -30°C, P(H2O)= 0 mbar	2019-05-27
	Verified	Unreleased	SPECTRUM_FAKE_2	New version v2 - Full spectrum 2 - NIR bidirectional reflection spectrum (i=0°/e=30°/az=0°) of Palagonite JSC Mars-1 with 5.07% adsorbed H2O at -30°C, P(H2O)= 4.0 10-5 mbar	2019-05-14
	Verified	Unreleased	SPECTRUM_FAKE_3	Full spectrum 3 - NIR bidirectional reflection spectrum (i=0°/e=30°/az=0°) of Palagonite JSC Mars-1 with 5.07% adsorbed H2O at -30°C, P(H2O)= 4.0 10-5 mbar	2019-05-14
	Verified	Restricted	SPECTRUM_BS_20181101_011	Vis-NIR reflectance spectra of 0.10% PAHs mixed with CO2 snow - 18-15mm	2018-11-13
	Verified	Restricted	SPECTRUM_BS_20181101_012	Vis-NIR reflectance spectra of 0.10% PAHs mixed with CO2 snow - 15-12mm	2018-11-13
	Unverified	Unreleased	SPECTRUM_BS_20181101_014	Vis-NIR reflectance spectra of 0.10% PAHs mixed with CO2 snow - xx-xx mm	2018-11-13
	Unverified	Unreleased	SPECTRUM_BS_20181101_015	Vis-NIR reflectance spectra of 0.10% PAHs mixed with CO2 snow - xx-xx mm	2018-11-13
	Unverified	Unreleased	SPECTRUM_BS_20181101_016	Vis-NIR reflectance spectra of 0.10% PAHs mixed with CO2 snow - xx-xx mm	2018-11-13
	Unverified	Unreleased	SPECTRUM_BS_20181101_017	Vis-NIR reflectance spectra of 0.10% PAHs mixed with CO2 snow - xx-xx mm	2018-11-13
	Unverified	Unreleased	SPECTRUM_BS_20181101_041	Vis-NIR reflectance spectra of 1.5% PAHs mixed with JSC Mars-1 dust	2018-11-13

# PID: the DOI in SSHADE

**DOI:** Unique identifier for

- SSHADE (*doi:10.26302/SSHADE*)
- each Database (*ex: doi:10.26302/SSHADE/GHOSST*)
- each Experiment (each version: TBD) (*doi: [10.26302/SSHADE/EXPERIMENT\\_BS\\_20121213\\_002.V1](https://doi.org/10.26302/SSHADE/EXPERIMENT_BS_20121213_002.V1)*)

**Automatically created (and upgraded)** using a set of KW of the datamodel:

- at database creation
- when an experiment is set to 'Public'

DOI redirects to a 'landing page'

**Information in DOI metadata:**

- **(ABS) Mandatory KW:** [Identifier](#), [Creators](#), [Title](#), [Publisher](#), [PublicationYear](#), [ResourceType](#)
- **Recommended KW:** subject, contributors (many types !), date, description, geolocation
- **Optional KW:** language, format, version, ...

**Data Reference:** Pommerol, A.; Schmitt, B. (2007): NIR bidirectional reflection spectrum of Smectite SWy-2 for different grain sizes at 298K. Version 1. SSHADE/GhoSST (OSUG Data Center). Dataset/Spectral Data. doi: [10.26302/SSHADE/EXPERIMENT\\_BS\\_20121213\\_002.V1](https://doi.org/10.26302/SSHADE/EXPERIMENT_BS_20121213_002.V1)

# Database manager: database management interface

- Database management

- ✓ Providers
- ✓ Providers import rights
- ✓ Members
- ✓ Link to experimentalist data

The screenshot displays the 'Database Manager' interface for the 'GhoSST' database. The interface is organized into several sections:

- Header:** Includes the 'Spectrum' logo, a search bar with the text 'Write your keywords here ...', and user information for 'Bernard Schmitt'.
- Navigation:** Tabs for 'Provider', 'Manager', and 'Admin' are visible. A sidebar on the left lists 'Databases', 'Experimentalists', and 'Groups', with 'Databases' selected.
- Database Details:** The 'Manager Database' section shows the acronym 'GhoSST' and the full name: '"Grenoble Astrophysics and Planetology Solid Spectroscopy and Thermodynamics" database service'. It includes 'Admin' and 'Add' buttons.
- Managers:** A section with an 'Admin' button.
- Providers:** A section with an 'Add' button and a table of providers. The table has columns for Family name, First name, Email, Access status, Access period, and Additional permissions. It shows 4 entries, all with an 'Authorized' status.
- Members:** A section with an 'Add' button and a table of members. The table has columns for Family name, First name, Email, Access status, and Access period. It shows 1 entry with an 'Authorized' status.
- Experimentalists:** A section with an 'Add' button.

Family name	First name	Email	Access status	Access period	Additional permissions
Schmitt	Bernard	bernard.schmitt@obs.ujf-grenoble.fr	Authorized	Always	import_correction, import_first
Garenne	Alexandre	alexgarenne@hotmail.com	Authorized	Always	
Rousseau	Batiste	batiste.rousseau@univ-grenoble-alpes.fr	Authorized	Always	import_correction, import_first
Quirico	Éric	eric.quirico@univ-grenoble-alpes.fr	Authorized	Always	import_correction

Family name	First name	Email	Access status	Access period
Schmitt	Bernard	Bernard.P.Schmitt@gmail.com	Authorized	Always

# Development of SSHADE VO

## Development of SSHADE Virtual Observatory (VO) access for VESPA

- Provide VO search on a limited number of main metadata
  - *species name/formula, compound type, object name, spectral type, T, P, grain size...*
- Allow to retrieve metadata and data for displaying in VO and associated tools/services
- Provide a link to the data in SSHADE (spectra in VOTable)

✓ Meeting (Nov. 2018) to define and implement a few new KW for better access and **search of laboratory data**

➔ implemented by VESPA in EPN-TAP

➔ **implemented in SSHADE**

➔ public VO completed and delivered last summer 2019



The screenshot shows the VESPA interface for the SSHADE service. It includes a search form on the left, a main content area with a description of the SSHADE spectra library, and a table of search results. On the right, there are plotting tools and example queries.

**SSHADE - SSHADE spectra library**  
SSHADE is an infrastructure for Solid Spectroscopy hosting a set of specialized databases provided by several research groups. SSHADE distributes spectral and photometric data (transmission, reflectance, optical constants, Raman, etc) obtained by various spectroscopic techniques over the whole electromagnetic spectrum but mostly covering the X, UV, Vis, Near/Mid/Far-IR, and sub-mm ranges. The measured samples include ices, minerals, rocks, organic, carbonaceous materials, and liquids — including field samples, synthesized and extraterrestrial materials. A dedicated search/visualization/export interface is available at <https://www.sshade.eu>. Information on SSHADE and its databases can be found at <https://wiki.sshade.eu/>

**Credits:**  
**Creators:** Damien Albert, Philippe Bollard  
**Contributors:** IPAG/CNRS, SSHADE partners, Bernard Schmitt  
**Publisher:** OSUG Data Center

Table of results:

granule_uid	dataprodut_type	target_name	time_min (d)
SPECTRUM_YD_20190911_060	cube		2010-02-16T00:00:00
SPECTRUM_YD_20190911_050	cube		2010-02-16T00:00:00
SPECTRUM_YD_20190911_040	cube		2010-02-16T00:00:00
SPECTRUM_YD_20190911_030	cube		2010-02-16T00:00:00

# Future SSHADE developments



# Future SSHADE developments

## **Europlanet-2024 RI (2020-2023)**

- Start: February 2020
- **VESPA work package**
  - SSHADE development: **band list of molecular solids**  
(+ extension of fundamental solids)
  - New partners => **new databases (8 - 12)**

## **Other needed developments**

- Multispectra visualization (internal comparison and with observations)
- BRDF : 4D multi-angle spectral and photometric visualization

# Bandlist of molecular solids

- **Bandlist:**

List of band parameters and vibration modes of an isotopic molecule

- in a simple constituent (2-3 species maxi)
- in a defined environment (T, P, ...)

- **Bands parameters**

- position (energy),
- width, shape, ...
- intensities (peak and integrated)
- accuracies / quality / evaluation

- **Transitions assignment**

- states QN, anharmonic coefficients, ...

➔ link to a constituent, mostly fundamental solid phases

- **Band parameters**

Variation of band parameters with temperature, pressure ...

- **Molecular vibration modes parameters**

Harmonic frequencies and anharmonic and interaction terms of molecular species in molecular solids

# Band lists and Bands

Home Search ▾ Data ▾ Producer ▾ Manager ▾ User ▾

GhoSST

Data / Bandlist / Bandlist / Bandlist / Bandlist / Bandlist / Bandlist

Bandlist Parameters Sample Primary constituent Publications Bands Copyright laboratories

### Bandlist

ID 37  
UID BANDLIST\_12CH4\_pure\_30K

#### Title and type

Title Band list of  $^{12}\text{CH}_4$  in pure  $\text{CH}_4$  ice I at 30K - Vis-NIR-MIR  
Type absorption band list  
Level 8

#### Origin and history

Date created 2001-06-14  
Date last updated 2013-08-09  
History 2013-01-21: new band list of 12CH4 in pure CH4 ice I at 30K - Vis-NIR-MIR

#### Sample, primary constituent and species

Sample CH4 crystalline I (SAMPLE\_BS\_20130114\_000)  
Material primary constituent CH4 crystalline - phase I (CONST\_BS\_20130114\_002)  
Constituent primary species (12C,1H4)Methane (MOLEC\_12CH4)

#### Variable parameters

Spectral unit cm-1  
Spectral standard vacuum

#### Analysis and validation

Analysis direct measurement on absorption coefficient spectrum  
Position reference 3010  $\text{cm}^{-1}$   
Quality flag 5  
Date validated 2001-06-14  
Validators

Show 10 ▾ entries Search:

ID	UID	Firstname	Lastname	Status	Laboratory
61	EXPER_Eric_Quirico_IPAG	Eric	Quirico	researcher	IPAG
67	EXPER_Bernard_Schmitt_IPAG	Bernard	Schmitt	researcher	IPAG

Showing 1 to 2 of 2 entries

#### References

Publication state published

#### Files

Filename bandlist\_12CH4-pureCH4icel-30K-NIR  
Original filename CH4-freq-table\_Grundy02.png

Documentation • Contact • History • Credits • Statistics

'old GhoSST':

- 15 bandlists
- 167 bands

Home Search ▾ Data ▾ Producer ▾ Manager ▾ User ▾

GhoSST

Data / Bandlist / Bandlist / Bandlist / Bandlist / Bandlist / Bandlist

Bandlist Parameters Sample Primary constituent Publications Bands Copyright laboratories

### Bands

Show 25 ▾ entries Search:

ID	UID	Peak position	Band width	Peak intensity ( $\text{cm}^{-1}$ )	Bond
122	BAND_12CH4_pure_30K_2598	2598	0	24.8	CH4
123	BAND_12CH4_pure_30K_2819	2819	0	133	CH4
124	BAND_12CH4_pure_30K_3010	3010	0		CH4
125	BAND_12CH4_pure_30K_3846	3846	0	48.4	CH4
126	BAND_12CH4_pure_30K_3897	3897	0	3.39	CH4
127	BAND_12CH4_pure_30K_4116	4116	0	9.59	CH4
128	BAND_12CH4_pure_30K_4203	4203	0	515	CH4
129	BAND_12CH4_pure_30K_4304	4304	0	267	CH4
130	BAND_12CH4_pure_30K_4530	4530	0	41.3	CH4
131	BAND_12CH4_pure_30K_5114	5114	0	0.19	CH4
132	BAND_12CH4_pure_30K_5162	5162	0	0.335	CH4
133	BAND_12CH4_pure_30K_5384	5384	0	1.43	CH4
134	BAND_12CH4_pure_30K_5566	5566	0	11.6	CH4
135	BAND_12CH4_pure_30K_5596	5596	0	5.7	CH4
136	BAND_12CH4_pure_30K_5800	5800	0	14.8	CH4
137	BAND_12CH4_pure_30K_5919	5919	0	2.54	CH4
138	BAND_12CH4_pure_30K_5990	5990	0	27	CH4
139	BAND_12CH4_pure_30K_6034	6034	0	7.59	CH4
140	BAND_12CH4_pure_30K_6616	6616	0	0.03	CH4
141	BAND_12CH4_pure_30K_6735	6735	0	0.649	CH4
142	BAND_12CH4_pure_30K_6858	6858	0	0.259	CH4
143	BAND_12CH4_pure_30K_6882	6882	0	0.286	CH4
144	BAND_12CH4_pure_30K_6999	6999	0	0.312	CH4
145	BAND_12CH4_pure_30K_7066	7066	0	2.83	CH4
146	BAND_12CH4_pure_30K_7084	7084	0	2.88	CH4

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Documentation • Contact • History • Credits • Statistics

# Band list

- Development/adaptation of bandlist datamodel
  - prototype already in GhoSST (to be adapted/modified to fit v0.9.0)
- Development of:
  - Bandlist database
  - Search tool / Visualization tool / Export interface
- Filling of the database

## **Review the available data for molecular solids**

- Partner's data (see examples in 'old GhoSST')
- Publications
  - => critical review and selection
  - => selection committee ? (→ 2020-22)

SSHADE is FAIR ?

## Findable

F1. (Meta)data are assigned a globally unique and persistent identifier

- ✓ *UID and DOI for a set of spectra (experiment') and their metadata*
- ✓ *UID for each spectra and its metadata*

F2. Data are described with rich metadata (defined by R1 below)

- ✓ *Various sets of metadata on sample, experiments, spectra, instruments, ...*

F3. Metadata clearly and explicitly include the identifier of the data they describe

- ✓ *UID and DOI are metadata of the experiment*

F4. (Meta)data are registered or indexed in a searchable resource

- ✓ *DOI registered at DataCite*

## Accessible

A1. (Meta)data are retrievable by their identifier using a standardized protocol

A1.1 The protocol is open, free, and universally implementable

✓ *DataCite DOI https protocol*

A1.2 The protocol allows for an authentication and authorization procedure

✓ ??

A2. Metadata are accessible, even when the data are no longer available

✓ *Data and metadata are persistently available, even when obsolete (old version) or discarded data (invalidated version)*

## Interoperable

I1. (Meta)data use a formal, accessible, shared, and broadly applicable language for knowledge representation.

- ✓ *SSDM datamodel common to the 20 databases of the SSHADE consortium. So some a largely shared language.*
- ✓ *Also interoperability developed with some VO (VESPA, VAMDC)*

I2. (Meta)data use vocabularies that follow FAIR principles

- ✓ ??

I3. (Meta)data include qualified references to other (meta)data

- ✓ *Reference to Publications (DOI, ...), data in other databases, ...*



## Reusable

R1. Meta(data) are richly described with a plurality of accurate and relevant attributes

R1.1. (Meta)data are released with a clear and accessible data usage license

X *Still missing ... (need agreement of all SSHADE partners...)*

R1.2. (Meta)data are associated with detailed provenance

✓ *Experimentalist/validator, instrument/laboratory, publications, ...*

R1.3. (Meta)data meet domain-relevant community standards

✓ *SSDM use as much as possible the standards of definition of solids, spectra, ..., but in crossing communities fields some tradeoff are made.*