

# 3<sup>rd</sup> SSHADE partners meeting

3-5 June 2019 – IPAG, Grenoble, France

EUROPLANET 2020-RI program  
VESPA JRA-5 + VA-2



# Aims of the 3<sup>rd</sup> SSHADE partners meeting

## **To present:**

- overall assessment of SSHADE activities during Europlanet-2020 RI
  - ✓ development of SSHADE interface
  - ✓ data provider trainings
  - ✓ current state of data ingestion in the SSHADE databases
  - ✓ documentation for providers and users
  - ✓ users: outreach & training, statistics of SSHADE use
- in-progress and last developments

## **To discuss and plan:**

- ✓ the last data ingestion rush before the final delivery of SSHADE
- ✓ SSHADE sustainability and issues: development/support and manpower
- ✓ individual databases sustainability, ...
- ✓ user training – advertising SSHADE
- ✓ what is intended in the future: Europlanet-2024 RI proposal, ...
- ✓ any question related to SSHADE and their databases

*SSHADÉ* and its activity

# 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)**
- ✓ **August 2019:** **SSHADE with 18-20 active databases (> 2500 spectra)**
  
- ✓ **Feb. 2020** **Europlanet-2024 RI ?**

# *SSHADÉ* European Consortium of Data Providers

Consortium of **23** solid spectroscopy experimental groups  
in **11** countries (F, GB, D, I, E, CH, PL, HU, AU, IN, TW)  
involving **~80** peoples

**Each with particular expertises on:**

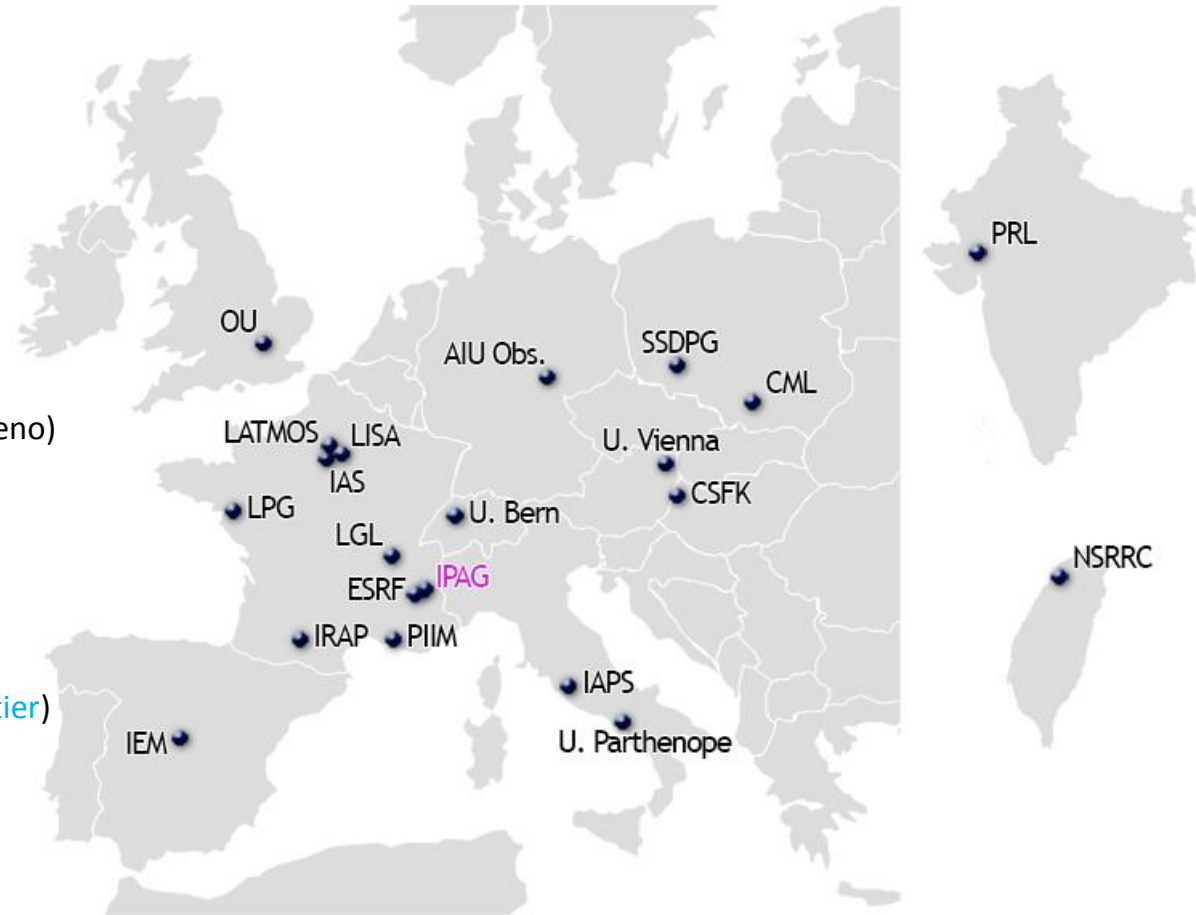
- some wavelength range
- specific techniques
- type of materials and physico-chemical conditions
- type of data and products, ...

**SSHADÉ wiki :** <https://wiki.sshade.eu/>

# The SSHADE-Europe consortium in EPN@2020-RI

**SSHADE (OSUG, Grenoble, F)** (Bernard Schmitt, Philippe Bollard, Damien Albert, Alexandre Garenne)

- **IPAG / Planéo**, Grenoble - F (Bernard Schmitt, Lydie Bonal)
- **Space & Planetary Science Division**, Univ. of Bern - CH (Antoine Pommerol, Olivier Poch, [Clément Feller](#))
- **IRAP / PEPS**, Toulouse - F (Patrick Pinet, Yves Daydou)
- **IRAP / MICMAC**, Toulouse - F (Karine Demyk, Yves Daydou)
- **SSDPG - Space Research Centre** – PL (Joanna Gurgurewicz)
- **IAS**, Univ. Paris-Sud - F (Rosario Brunetto, Donia Baklouti)
- **LPG**, Univ. Nantes - F (Marion Massé, Manuel Giraud)
- **AIU Observatory**, Jena - D (Harald Mutschke, Jürgen Weiprecht)
- **ESRF / FAME line**, Grenoble – EU / F (Denis Testemale, Isabelle Kieffer)
- **Clay Mineral Laboratory**, Institute of Geological Sciences – PL (Artur Kuligiewicz)
- **PIIM**, Univ. Aix-Marseille - F (Patrice Theulé)
- **Instituto de Estructura de la Materia**, Madrid – E (Vicente Timón, Miguel Angel Moreno)
- **Open University**, Milton Keynes – UK (Nigel Mason)
- **PRL**, Ahmedabad – IN (Bhala Sivaraman, [Bhushit Vaishnav](#), [Dinesh Mehta](#))
- **LISA**, Univ. Paris-Est - F (Nicolas Fray)
- **Centro de Astrobiología**, INTA-CSIC – E (Guillermo Muñoz Caro)
- **LATMOS / IMPEC**, Institut Pierre Simon Laplace - F (Nathalie Carrasco, [Thomas Gautier](#))
- **IAPS**, INAF, Roma - I (Alessandra Rotundi, [Andrea Longobardo](#), Vincenzo della Corte)
- **IAPS**, INAF, Roma - I (Fabrizio Capaccioni, Christian Carli)
- **LGL / ENS-Lyon** - F (Bruno Reynard, Gilles Montagnac, Razvan Caracas)
- **Konkoly Astronomical Institute** – HU (Akos Kereszturi, Ildiko Gyollai)



# Euromlanet 2020-RI JRA-5 Activities (WP 11)

**JRA – SSHADE infrastructure development** → **delivered 1st February 2018**

## **Databases infrastructure**

- Continuation of development and upgrade of interface (Year 3 - 4)
- Major upgrade of SSDM (data model) (Year 4)
- Major upgrade of the imported data (Year 4)
- DOI workflow implementation (Year 4)
- Consolidation of the system infrastructure (Year 4)
- Development of the common 'band list database' (Years 3 - 4)

## **VO interoperability**

- Interop with VESPA-VO and VAMDC-VO (years 3- 4)

# Euromlanet 2020-RI

## VA-2 Activities (WP 6)

### VA – Database feeding

→ delivery every year up to August 2019

#### Coordination of consortium

- Preparation and feeding of the common fundamental data of SSHADE (Year 3)
- Development of the common 'band list database' (option Years 3 - 4)

#### Support to consortium

- Final SSHADE consortium meetings (Year 4)
- Formation/training of database managers and 'providers' (Year 3)
- Preparation of documentations and tutorials for providers (Year 3)
- In-situ & on-line support to each database manager (Year 3 - 4)

#### Support to users

- Tutorials & training for users at conferences (Years 3 - 4)
- Preparation of documentations and tutorials for users (Years 3 - 4)

#### Partners

- Preparation and feeding of spectral data and metadata (Years 3 - 4)



# SSHADE events Time line

## 2017

- December

2nd SSHADE meeting

## 2018

- January
- January
- March
- May-June-July
- August
- September
- October
- October
- December

8 active + 2 starting databases in SSHADE

**SSHADE infrastructure delivery**

(D11.7 JRA VESPA)

Training users ELS

Training database managers + SSHADE-Parties

11 active + 3 starting databases in SSHADE

(D6.3 VAA VESPA – Y3)

Training users EPSC

(D6.5 VAA VESPA – Y3)

Training database managers

Training users DPS

SSHADE-Party

## 2019

- May
- June
- July
- July
- August
- August
- September

**Major upgrade of SSHADE infrastructure and data (v0.9.0)**

3rd SSHADE meeting

Training users Pluto conference

≥ 18 active databases in SSHADE

**SSHADE with 18-20 active databases**

(D6.3 VAA VESPA – Y4)

End of Europlanet 2020-RI

(D6.5 VAA VESPA – Y4)

Training users EPSC-DPS

# 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'](#) (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 (to be completed)
- Inclusion of field and airborne measurements
- Addition of geolocation of natural samples (collected or field measurement)

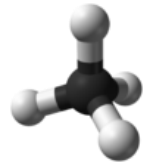
- **Spectra:**

- Better description and import of multi-angle data (BRDF, ...)
- Improvement of experiment/spectra version management
- Addition of several preview options for experiment and spectra
- Extension of the spectral range and spectrum types to radio wavelength
- Extension to Polarized spectra (but not yet specific import format for set of 4 parameters)
- 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, ... ..

# Planetary objects and bodies (v 0.9.0)



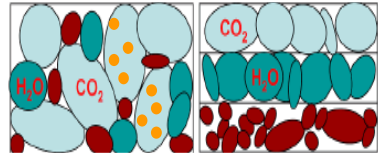
SPECIES

PHASES

MATTERS

OBJECTS

BODIES



SAMPLE

INSTRUMENT



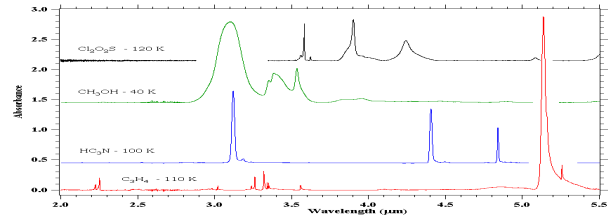
EXPERIMENT

PROVIDER



BAND LIST

SPECTRA



JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 105, NO. E11, PAGES 2489-2502, OCTOBER 15, 1998

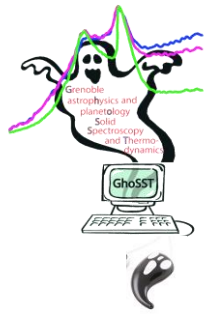
The temperature-dependent near-infrared absorption spectrum of hexagonal H<sub>2</sub>O ice

W. M. Grundy<sup>1</sup> and B. Schmitt  
 CNRS/Laboratoire de Glaciologie et Géophysique de l'Environnement, Grenoble, France

**Abstract.** Transmission spectra were measured between 1.0 and 2.7 µm for microcrystalline samples of hexagonal water ice at temperatures between 20 and 270 K. Samples were crystallized from liquid water within closed cells with thicknesses ranging from 100 µm to 1.0 cm. The absorption spectrum of ice changes with temperature in several ways. With higher temperature, the shape of absorption bands shifts to shorter wavelengths, the shape of absorption bands becomes more smoothed, the strength of some absorption bands decreases, the absorption in continuum wavelengths increases, and the band centers of some absorption bands shift to shorter wavelengths. In this paper we present the new absorption coefficient spectra along with an examination of the different temperature effects. These data should prove extremely valuable for analysis of near-infrared reflectance spectra of low-temperature icy surfaces, such as those of outer solar system satellites, Kuiper Belt objects, Pluto and Charon, comet nuclei, the polar caps of Mars, and terrestrial snow- and ice-covered regions. The data may also be of value in simulating radiative transfer in clouds of ice particles in the atmospheres of planets.

Wavelength (µm)	Wavenumber (cm <sup>-1</sup> )	Band Name
1.0	10000	OH stretch
1.2	8333	OH stretch
1.5	6667	OH stretch
1.8	5556	OH stretch
2.0	5000	OH stretch
2.2	4545	OH stretch
2.5	4000	OH stretch
2.8	3571	OH stretch
3.0	3333	OH stretch
3.2	3125	OH stretch
3.5	2857	OH stretch
3.8	2632	OH stretch
4.0	2500	OH stretch
4.2	2381	OH stretch
4.5	2222	OH stretch
4.8	2083	OH stretch
5.0	2000	OH stretch
5.2	1923	OH stretch
5.5	1818	OH stretch

PUBLICATIONS



# Planetary objects and bodies (v 0.9.0)

- **Planetary bodies** (New):

Describe planetary objects on which material, rocks, ... (called 'planetary object') are collected by space missions

- Earth, Moon, Mars, 81P/Wild, Itokawa, Ryugu, Bennu, ...



- **Planetary objects** (New, TBC):

Describe planetary material, rocks, grains,... collected by space missions :

- Moon (Apollo, Luna, ...), Asteroids (Hayabusa 1-2, OSIRIS-REX, ...), Comets (Stardust, ...), ...
- Link to « Body »

=> **Draft to be completed**,  
and implemented before use  
for importing planetary matters

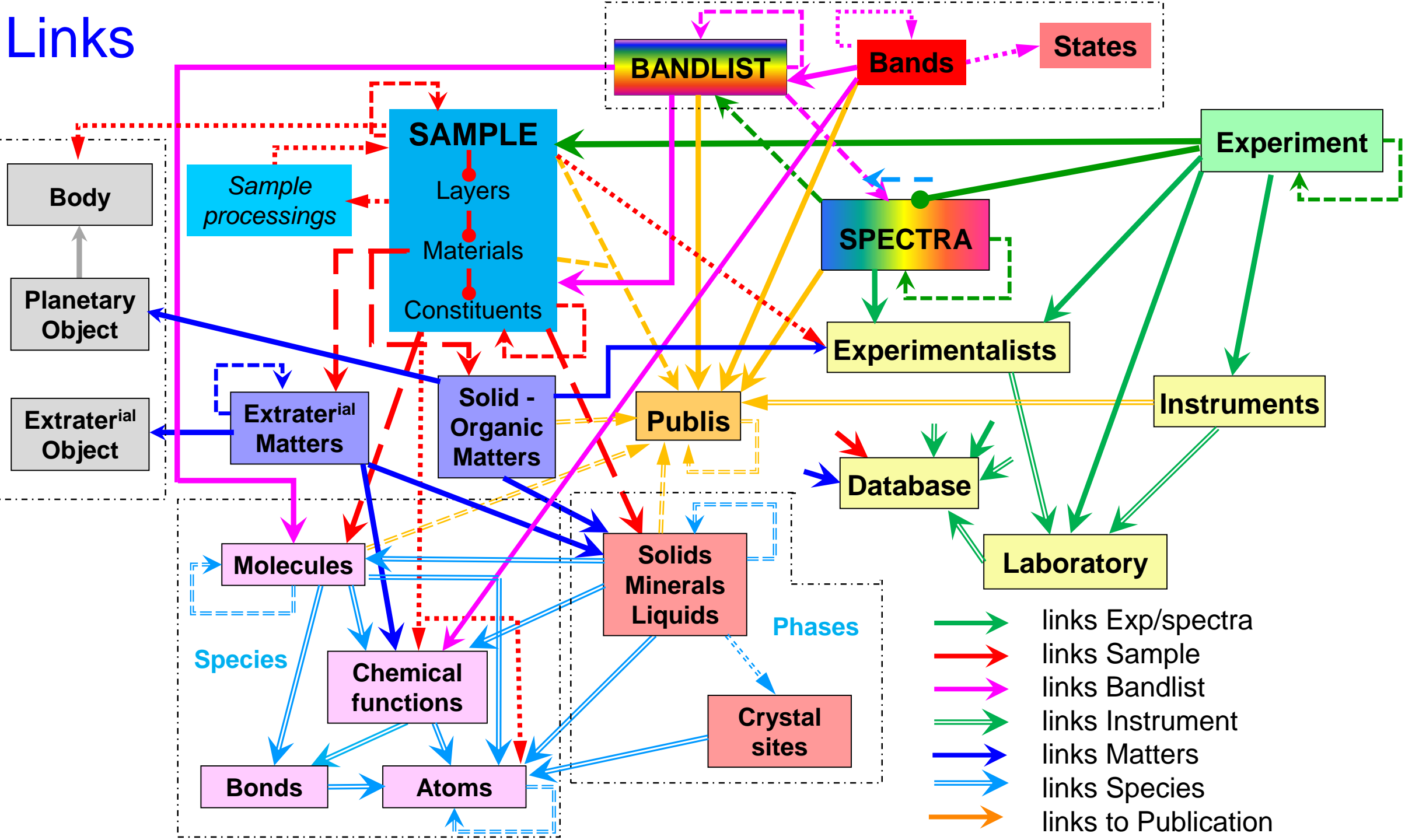
**Will be prepared by SSHADE (on request)**



The screenshot shows the SSHADE web interface for a 'Planetary body' named 'Moon'. The interface includes a header with the SSHADE logo and a menu icon. Below the header, there are several sections with expandable/collapsible headers, each with a red downward arrow icon:

- Planetary body** (with ID and UID buttons)
- Name**: Moon
- Secondary names**: Luna, Selene
- Origin**
- Family and type**
- Orbit**
- Rotation**
- Physical properties**
  - Mean radius**: 1737.1 km
  - Mass**: 0.0123 kg (0.001 Earth mass)
  - Mean density**: 3.344 g/cm<sup>3</sup>
  - Surface**
    - Gravity**: 1.62 m/s<sup>2</sup>
    - Geometric albedo (Vis)**: 0.12
    - Bond albedo**: 0.136
    - Temperature**: 100 - 390K (equator)
    - Pressure**: outgassing and sputtering atmosphere: 110<sup>-12</sup> mbar (night) - 110<sup>-9</sup> mbar (day)
- Composition**
- Links**

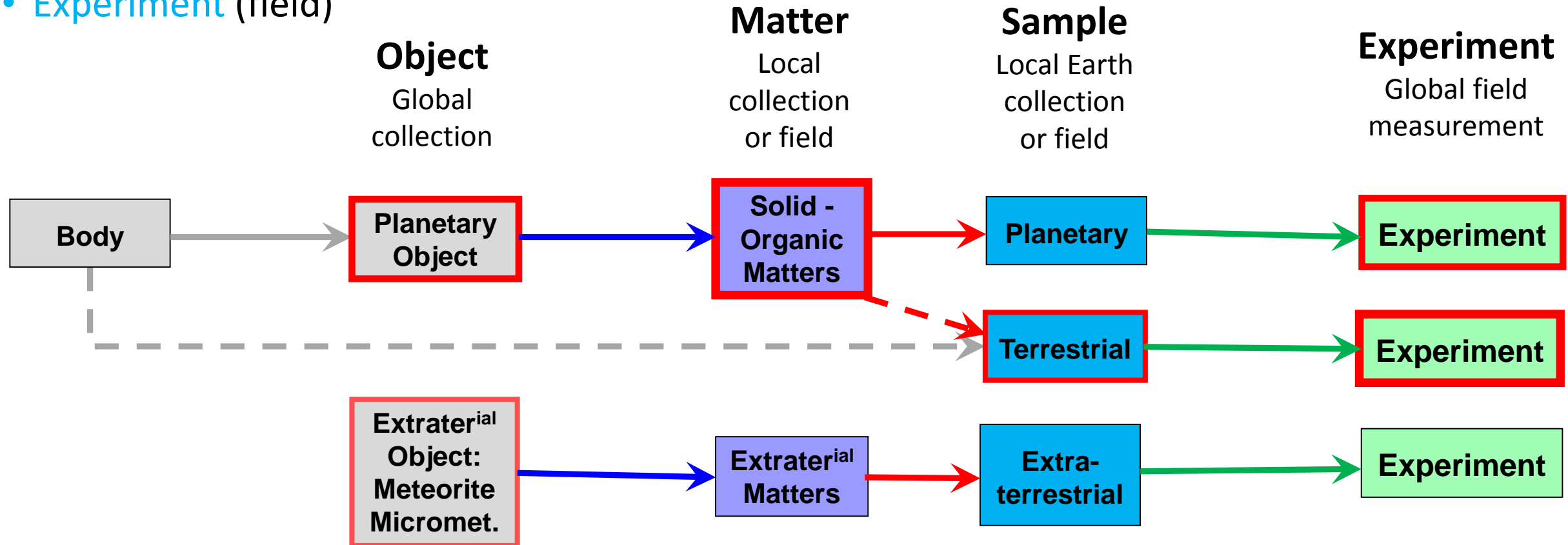
# Links



# 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 data (v 0.9.0)

- **Spectra:**

Splitting of « spectrum\_type » in 3 keywords:

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

Reorganization of file import with 4 options depending on dataset organization in file(s):

- unique file containing a full spectro-photometric data set (BYPASS, GhoSST...)
- series of spectrum files at single geometry in a multi-angle dataset (GhoSST, ...)
- 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 (PaSSTEL, ...)

**→ all data are homogeneously stored in the same database structure at 4 dimensions**

+ 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)

➔ Flag on spectra to tell if obsolete/invalidated and when a new version exists

The screenshot displays the SHADE web interface. At the top, there is a search bar with the text 'Spectrum' and a search icon. Below the search bar, the main content area is divided into two panels. The left panel, titled 'Experiment and spectra', shows a tree view of the experiment 'FULL experiment - v1'. It contains two sub-experiments: 'sample thickness 1' and 'emergence angle 1'. Each sub-experiment has three associated spectra: 'Full spectrum 1', 'Full spectrum 2', and 'Full spectrum 3'. The right panel, titled 'Spectrum history', shows the history for the selected spectrum. It includes fields for 'Experiment', 'Parent spectrum', 'Date begin', 'Date end', 'Release date', and 'Version (Date)'. Below these fields is a table with the following columns: 'Date', 'Mode', 'Version', 'Status', and 'Comments'. The table contains several rows of data, including dates, modes (import, correction, new version), version numbers, and status indicators (obsolete, partly invalidated, valid).

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 (2019...)

- **Planetary objects :**

- Only option still to be completed !
- and implemented before fully importing planetary matters (except terrestrial)

## **No other options and changes planned in SSDM ...**

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

- Implementation of 4-parameters polarization import and storage (2020..., when format defined)
- Implementation of n-entries model parameters import and storage (when ?)
- Implementation of spectro-images import and storage (later ...?)
- Bandlists (upgrade from GhoSST) + band parameters and [future Europlanet-2024 RI]

# SSDM + SSHADE DB implementation

	<u>SSDM</u>	<u>SSHADE</u>
• Databases/Laboratories/Experimentalists:	→ Stable	Done
• Species:		
– Atomic and Molecular	→ Stable	Done
– Chemical bonds and functions	→ Stable	Done
• Phases:		
– Minerals	→ Stable	Done
– Solids, Liquids	→ Stable	Done
• Matters:		
– Fluids	→ Stable	Done
– Solids	→ Stable	Done
– Extraterrestrial	→ Stable	Done
– Carbonaceous	→ Stable	Done
• Objects:		
– Meteorites, Micrometeorites, IDPs, <b>Planetary</b>	→ Stable/TBC	Done
• Bodies	→ Stable	Done
• Samples: Layers/Material/Constituents	→ Stable	Done
• Instruments/techniques:	→ Stable	Done
• Spectra and products:	→ Stable	Done
• Publications	→ Stable	Done

# Development of SSHADE interface

# Development of SSHADE interface

A lot of new features and tools since last meeting !!!

- 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, ....

- ➔ Questions/discussion on SSHADE interface
- ➔ Discussion on interface testing

# User: Search interface

- **Search :**

- ✓ more efficient top search bar
- ✓ More efficient operators (*is, contain any, contain all, wildcard, ...*)
- ✓ more filters choice
- ✓ Reset modes: global, per keyword
- ✓ ...

- **Results :**

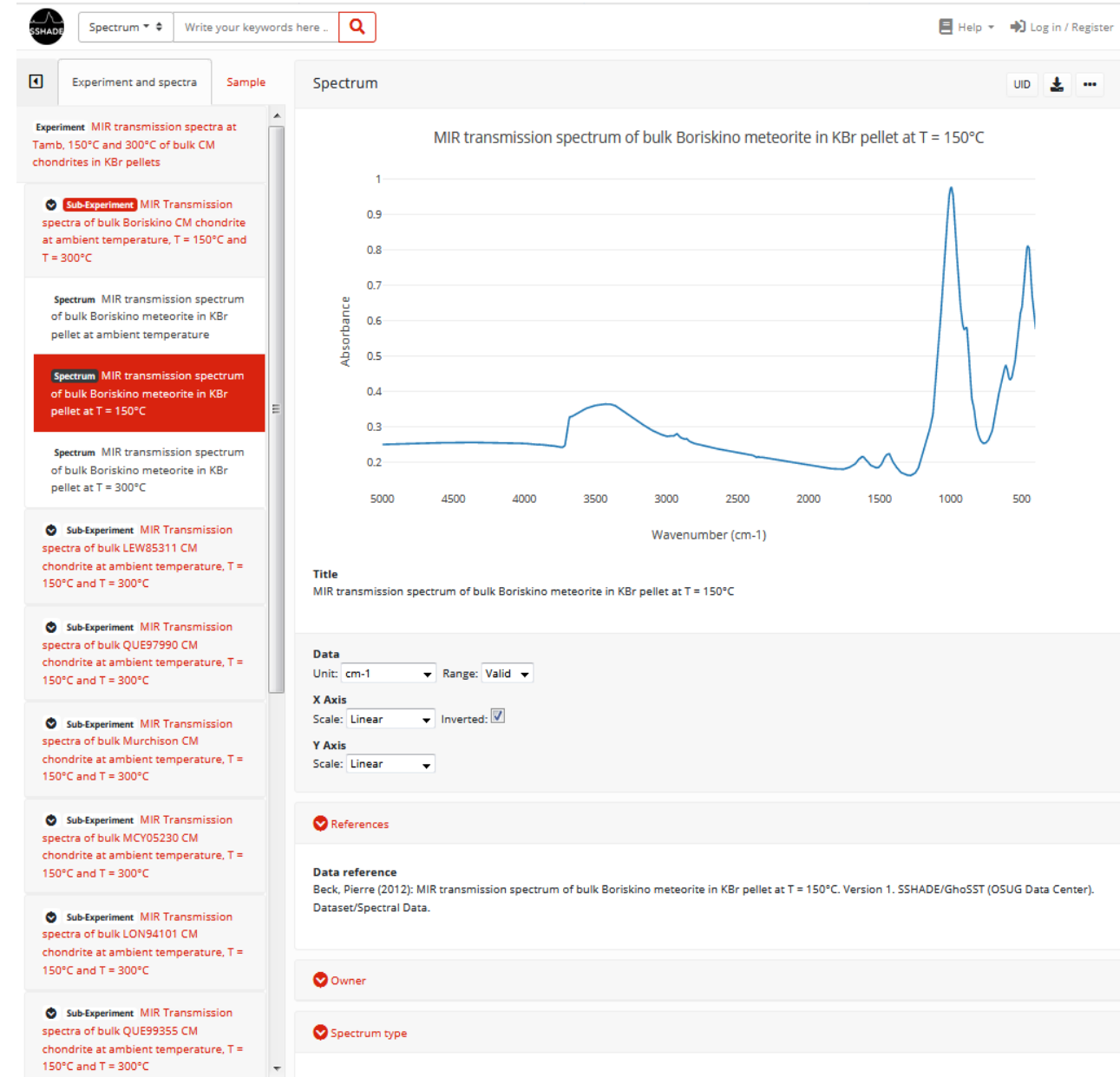
- ✓ Well working experiment grouping

The screenshot displays the SHARD 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 "By instrument parameters" category is expanded, showing various filters such as "Technique", "Spectral", "Polarization", and "Angular". The "Spatial" filter is currently selected, and a dropdown menu is open, showing a list of options: "macroscopic", "microscopy", "linear scan", "linear micro-scan", "imaging", and "micro-imaging". The "microscopy" option is highlighted in red and has a checkmark next to it. The interface also includes a "Filters" section with a "Reset all filters" button and a "Spectra search" section with a "Reset" button.

# User: Experiment-spectra / Sample data interface

- **Experiment display :**

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

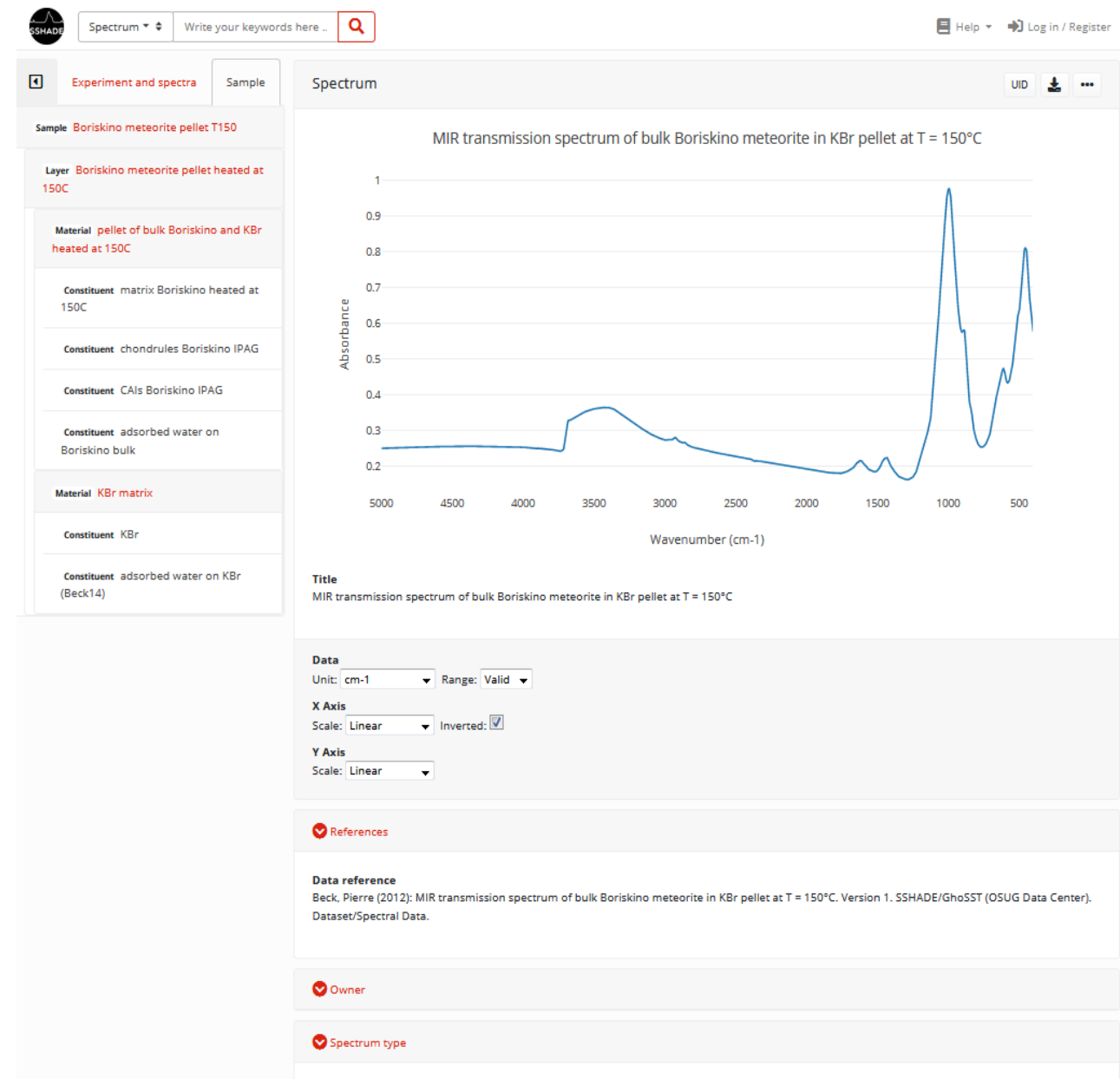




# User: Experiment-spectra / Sample data interface

- **Experiment display :**

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



# User: Experiment-spectra / Sample data interface

- **Experiment display :**

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

- **Samples :**

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

The screenshot displays the SSHADE web interface. At the top, there is a search bar with the text "Write your keywords here ..." and a search icon. The interface is divided into two main sections: "Experiment and spectra" and "Sample".

**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)

**Constituent:** matrix Boriskino heated at 150C

**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

**Constituent abundance in material:** (checked)

**Chemical composition:** (checked)

**Species:** (checked)

	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 listing export records with columns for Export, UID, Title, Export date, Size, Steps, Progression, and ETA.

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 listing import records with columns for Date and Source file.

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: verification / release interface

- **Unverified data**

- ✓ Experiments / spectra
- ✓ Unverified/verified status
- ✓ Verification process
- ✓ Also from data page

- **Unreleased/Restricted data**

- ✓ Experiments / spectra
- ✓ Private / Restricted / Public status
- ✓ Publication process
- ✓ Also from data page

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 tabs for "Provider", "Manager", and "Admin". The "Provider" tab is active, and the page title is "Provider Unreleased/Restricted spectra".

The main content area shows a table of 12 entries. The table has columns for "Status", "Access", "UID", "Title", and "Imported". Each entry has a "Show" button (eye icon) and a "Verify" button (checkmark icon). The "Status" column shows "Verified" (green) or "Unverified" (purple). The "Access" column shows "Unreleased" (purple) or "Restricted" (blue). The "UID" column shows the unique identifier for each spectrum. The "Title" column shows the description of the spectrum. The "Imported" column shows the date when the spectrum was imported.

Show	Status	Access	UID	Title	Imported
	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

At the bottom of the table, there is a pagination bar showing "Showing 1 to 10 of 12 entries" and navigation buttons for "Previous", "1", "2", and "Next".

# 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:** Shows the 'Acronym' as 'GhoSST' and the 'Name' as '"Grenoble Astrophysics and Planetology Solid Spectroscopy and Thermodynamics" database service'.
- 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 lists four providers: Schmitt, Garenne, Rousseau, and Quirico, 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 lists one member: Schmitt, with an 'Authorized' status.
- Experimentalists:** A section at the bottom with an 'Add' button.

# Development of SSHADE interface

- Feedback on SSHADE interface
- Questions/discussion on SSHADE interface
- Interface testing

Provider developments of XML convertors



# Data provider: data convertors to xml

- **Data convertors**

**A few databases have developed customized convertors from simple standardized user files to xml files :**

- Sample, Matter ?
  - Experiment-spectra
  - Experimentalist, laboratory, ... ?
- 
- ✓ FAME                      Isabelle Kieffer    (=> presentation)
  - ✓ SSTONE                  Manuel Giraud    (=> presentation)
  - ✓ ACID                      Dinesh Metha, ...
  - ✓ Others ? ...

**➔ Interested for sharing such developments ?**

# Data provider: data converters to xml

- **Simple web xml file generators ?**

**for the simplest provider xml files:**

- Publication => BibTeX convertor @ SSHADE import
- Database,
- Experimentalist, Laboratory → the most useful for external experimentalists !
- Instrument → useful when using external instrument/facility

**for the simplest SSHADE xml files:**

- Molecules, Fundamental phases ?
- Objects (Meteorite, ...) ?

**Discussion: Which specific interest ?**

- For members, internal/external experimentalists (experimental facility, ...) ?

# Development of SSHADE VO

# 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 the data (spectra in VOTable) for displaying in VO and associated tools/services
  - with a few metadata for info in VO
  - Provide a link to the data in SSHADE
- ✓ Meeting (Nov. 2018) to define and implement a few new KW for better access and search of laboratory data, on solids in particular
- ➔ recently implemented by VESPA in EPN-TAP
  - ➔ **will be implemented soon in SSHADE**
- ➔ **VO will be completed, tested and delivered by this summer**

# The DOI in SSHADE

# The DOI in SSHADE

**DOI:** Unique identifier for

- SSHADE *(doi:10.17178/SSHADE)*
- each Database *(ex: doi:10.17178/SSHADE/GHOSST)*
- each Experiment *(see next slide)*

**Information in DOI metadata:**

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

# The DOI in SSHADE

## DOI for Experiment:

- doi:10.17178/SSHADE/EXPERIMENT\_BS\_20121213\_002.V1

The most important KW: « experiment\_uid »

=> follow UID creation rule!

(‘EXPERIMENT\_AB\_yyymmdd\_nnn’)

## Mandatory Meta data & Data citation:

- Creators (PublicationYear): Title. Version. Publisher. ResourceType. Identifier

### The used KWs:

- Creators = List of « experimentalist\_names + validator\_names » => list all them!
- PublicationYear = year when data are put on-line (public) « experiment\_date\_released»
- Title: « experiment\_title » => choose it carefully (fully explicit about content and readable) !
- Publisher = SSHADE/« experiment\_owner\_database » (OSUG Data Center)
- ResourceType = ‘Dataset/Spectral Data’ (fixed)
- Identifier = DOI (from « experiment\_uid »)

**Example:** *Think as for a Journal paper 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: [10.17178/SSHADE/EXPERIMENT\\_BS\\_20121213\\_002.V1](https://doi.org/10.17178/SSHADE/EXPERIMENT_BS_20121213_002.V1)

# The DOI in SSHADE

## How it is created:

will be automatically created using a set of KW:

- at database creation (action to be defined)
- when an imported and validated experiment is set to 'Public'

## How it will work:

DOI will redirect to a 'landing page'

=> database page @ SSHADE

=> the experiment page @ SSHADE (with a warning if there is a new version or invalidated data)

➔ will be implemented soon (still waiting signed contract back from university ...)

➔ we will process for creation of the DOIs of a database only when the Scientific Manager can guaranty all « experimentalist » list and « experiment title » of their public data have been checked.



# The SSHADE Wiki

# The SSHADE Wiki

<https://wiki.sshade.eu>

## By SSHADE team

- XML import templates (up-to-date v0.9.0) : OK
- SSDM data model: to clean v0.9.0
- Documentation for providers: Import manual, tutorials, ... : to be updated v0.9.0
- Documentation for the user (user manual, citation rules): OK

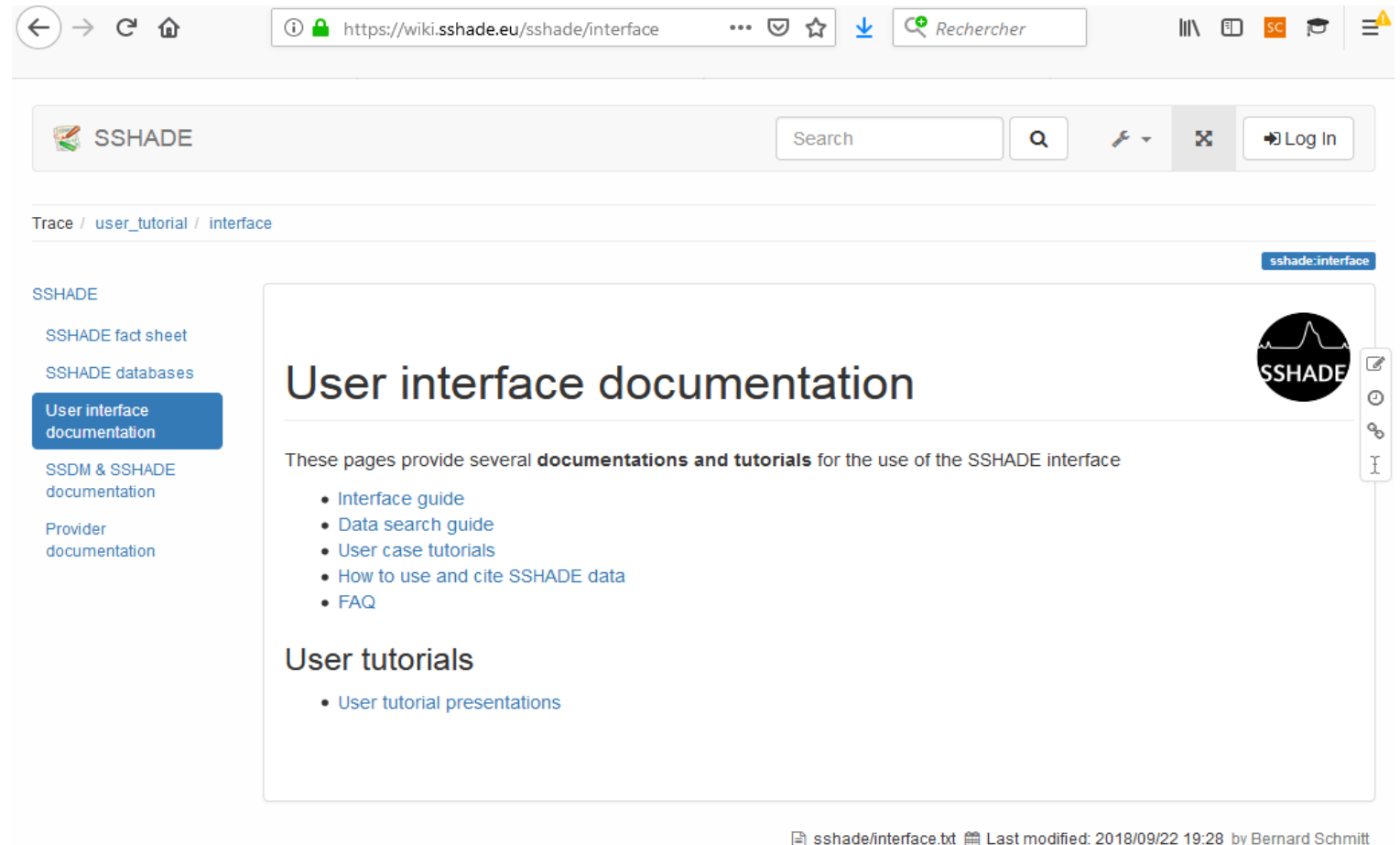
## By each partner

- Description for all databases: samples, instrument-techniques  
→ to be completed by a few databases (ISMAD, MIA, MTACSFK, REFL\_SLAB, RSPS, SCOOP, SPAN)

# Document for users

- SSHADE wiki: <https://wiki.sshade.eu/ssshade/interface>

- Interface guide
- Data search guide
- User case tutorials  
(old: GhoSST)
- How to use and cite  
SSHADE data
- FAQ
  
- User tutorial presentations



The screenshot shows a web browser displaying the SSHADE wiki page for user interface documentation. The browser's address bar shows the URL <https://wiki.sshade.eu/ssshade/interface>. The page header includes the SSHADE logo, a search bar, and a 'Log In' button. The breadcrumb trail is 'Trace / user\_tutorial / interface'. The main content area is titled 'User interface documentation' and contains a list of links: 'Interface guide', 'Data search guide', 'User case tutorials', 'How to use and cite SSHADE data', and 'FAQ'. Below this, there is a section for 'User tutorials' with a link to 'User tutorial presentations'. The footer of the page indicates the file is 'ssshade/interface.txt', last modified on 2018/09/22 at 19:28 by Bernard Schmitt.

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# Data ingestion in SSHADE and its databases

# State of data ingestion in SSHADE and its databases

- SSHADE

- Fundamental Species:
  - ✓ Atoms, molecules, chemical bonds, chemical functions
- Fundamental Phases:
  - ✓ minerals, solids, liquids
- Reference Matters
- Objects, Bodies
  - ✓ Meteorites, Cosmic Dusts, IDPs, Earth/Moon
- Publications, Journals

- SSHADE databases

- Database, laboratory, experimentalists, Instruments-techniques
- Local Matters, Samples
- Experiments & Spectra
- Publications

# State of data ingestion in SSHADE and its databases

*Dec. 2017 => June 2019*

## Species

- Atoms 141 => 148
- Chemical bonds 192 => 205
- Chemical Functions 51 => 56
- Molecules 116 => 149

## Phases

- Minerals 169 => 177
- Solids 46 => 98
- Liquid 8 => 10

## Objects

- Meteorites 94 => 108
- Micrometeorite 11 => 11
- IDPs 0 => 3

## Bodies

0 => 2

**TOTAL** 828 => 967

*Dec. 2017 => June 2019*

## Databases

- Databases 12 => 21
- Laboratories 34 => 60
- Experimentalists 72 => 136
- Instruments-techniques 82 => 103

## Matters

- Fluid 38 => 38
- Solid 57 => 114
- Mineral 64 => 66
- Carbonaceous 4 => 14
- Extraterrestrial 59 => 88

## Publications

- Journals 44 => 59
- Publications 174 => 262

**TOTAL** 640 => 961

# State of data ingestion in SSHADE databases

Database	Matters	Samples	Experiments	Spectra
ACID		4	1	2
BYPASS	4	16	3	76
COMEDA		3	1	3
CSS		4	1	9
DAYSY	2	11	17	82
DOCCD	11	62	7	56
FAME	8	82	72	154
GhoSST	86	377	56	516
ISMAD		2	1	4
LSD	63	130	33	145
MIA	0	10	5	6
MTACSFK		1	1	1
PaSSTEL	15	12	13	18
REFL_SLAB		18	4	116

Database	Matters	Samples	Experiments	Spectra
RSPS		4	1	4
SCOOP		34	2	34
SOSYPOL	2	73	18	315
SPAN		15	5	20
SSTONE	6	370	7	370
STOPCODA	14	12	3	56
<b>Total</b>	<b>211</b>	<b>1270</b>	<b>251</b>	<b>1987</b>

20 Databases:

- Samples
- Experiments
- Spectra

*Dec. 2017 => June 2019*

797 => 1240

156 => 251

1231 => 1987

**TOTAL**

2184 => 3478

**GRAND TOTAL**

3652 => 5406 files

# Conversion of all imported data in v0.9.0

## Changes in xml files:

- few modified/improved structures (*spectrum\_file, ...*)
- new mandatory keywords (*spectral/angle\_observation\_mode, material\_relevance...*)
- some new options (*spectrum version, geolocation, preview, ...*)
- some changes/additions in Enum attributes (*experiment\_type, spectrum\_type, ...*)

→ in all former files (old versions)

## Testing import in v0.9.0:

→ replay import, with all corrections, new versions (history preserved)

## Final import of v0.9.0 archive

→ zip with over 10 000 files !

→ success !!!



# Conversion of all imported data in v0.9.0

## xml files stored in SSHADE:

- complete in v0.9.0
- added important options to all (*new version of spectra, ...*)

*but*

- missing some new options => **add them if needed**
- some attributes of KW set to a default value or to NULL => **need to be verified / completed**
- some defect in xml structuration
- not all Enum lists up-to-date
- not all comments up-to-date

➔ refer to the **last XML templates v0.9.0** (WIKI: <https://wiki.sshade.eu/ssshade/provider/templates>)

➔ need to have **clean specialized templates in v0.9.0**

- for each type of experiment
- for each database

➔ In process by SSHADE team for 1-3 specialized template per database

➔ need to have a **short tutorial on v0.9.0** (on-line) before restarting to import

# Partner's training

# Initial partner's training

Trained partners between Dec. 2017 and Dec. 2018

8 last partners trained (+ SSHADE party):

- SCOOP                      LISA (Créteil, F)                      => Paris, May + Dec 2018
- SPAN                        LATMOS (Guyancourt, F)              => Paris, May + Dec 2018
- COMEDA:                  IAPS (Roma, I)                        => Roma, June + Nov. 2018
- REFL\_SLAB                IAPS (Roma, I)                        => Roma, June + Nov. 2018
- ISMAD:                    IEM (Madrid, E)                       => Grenoble, Juillet 2018
- MTACSFK                  CSFK (Budapest, HU)                => Grenoble , Juillet 2018
- ACID:                      PRL (Ahmedabad, IN)                => Ahmedabad, Oct. 2018
- RSPS                        LGL-TPE (Lyon, F)                    => Lyon, Nov. 2018

# Partner's 'SSHADE Party'

## How

- 1-2 full days at partner lab or in Grenoble, or on-line

## Aim

- Help to prepare and ingest one set of data for the different types of sample / experiment
- Build specialized matter / sample / experiment templates for these types of experiments

## Outcome

- Seems to have strongly helped and motivated the partners for data ingestion.
- **Need Your feedback !**

# Partner's training for v0.9.0

## Training content

- ✓ explanation of the v0.9.0: **SSDM and XML changes** and their impact on your data.
- ✓ provision of a fully **up-to-date and documented specialized xml template** for your different data types  
(selection by you and preparation by us a few days before)
- ✓ supervised **completion/verification by you of a few new/modified KW** in your xml files  
(database, matter/sample/experiment-spectra)
- ✓ if possible: preparation by you of **a new set of data** under our supervision (online or by mail)
- ✓ **Answer your questions** on the new version (or any other)

# Partner's training for v0.9.0

## Training planning

~ Half a day

3 done, 11 planned

Still some free dates :

- 20, 24-28 June
- 3-5 July

➔ Still awaiting the answer of 5 databases.

MIA	P. Theulé	16-may
FAME	I. Kieffer, D. Testemale	23-may
BYPASS	C. Feller	31-may
SPAN	Th. Gautier	06-june
LSD	A. Kuligiewicz	07-june
DOCCD	H. Mutschke	14-june
SSTONE	M.Massé, M. Giraud	17-june
SOSYPOL	J. Gurgurewicz	18-june
DAYSY	D. Baklouti	19-june
SCOOP	N. Fray	25-June
MTACSFK	A. Kereszturi, I. Gyollai ?	25/6-3/7, 5/7
BYPASS	O. Poch	08-july
PaSSTEL	Y. Daydou, P. Pinet	09-july
STOPCODA	K. Demyk	10-july
ACID	D. Mehta ?	?
COMEDA	A. Longobardo	?
ISMAD	V. Timon, M.A. Moreno	?
REFL_SLAB	C. Carli	?
RSPS	G. Montagnac	?

Planning data feeding by partners

# State of data ingestion in SSHADE databases

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20 Databases:

- Samples
- Experiments
- Spectra

*June 2019*

1240

251

1987

public: 1490 spectra



# State of data ingestion in SSHADE databases

Database	Matters	Samples	Experiments	Spectra
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SSTONE	6	370	7	370
STOPCODA	14	12	3	56
<b>Total</b>	<b>211</b>	<b>1270</b>	<b>251</b>	<b>1887</b>

## 20 Databases:

- 11 Actives
- 2 being active
- 7 starting
- But the long 'import stop' for v0.9.0 upgrade is probably the main reason

# Database feeding by partners

- 1) before end of summer

June – July – (August)

**Aim 1: at least 18 active databases** (with more than ~ 50 spectra per DB)

**=> Success !**

**Aim 1: at least 2500 public spectra** (currently ~1500 public + ~500 private)

=> report of SSHADE in Final Europlanet report (end july)

- 2) after summer

Continue at your pace !

# SSHADE events Time line

## 2017

- December

**2nd SSHADE meeting**

## 2018

- January
- January
- March
- May-June-July
- August
- September
- October
- October
- December

8 active + 2 starting databases in SSHADE

**SSHADE infrastructure delivery**

**(D11.7 JRA VESPA)**

Training users ELS

Training database managers + SSHADE-Parties

11 active + 3 starting databases in SSHADE

**(D6.3 VAA VESPA – Y3)**

Training users EPSC

**(D6.5 VAA VESPA – Y3)**

Training database managers

Training users DPS

SSHADE-Party

## 2019

- May
- June
- July
- July
- August
- August
- September

**Major upgrade of SSHADE infrastructure and data (v0.9.0)**

**3rd SSHADE meeting**

Training users Pluto conference

≥ 18 active databases in SSHADE

**SSHADE with 18-20 databases**

**(D6.3 VAA VESPA – Y4)**

**End of Europlanet 2020-RI**

**(D6.5 VAA VESPA – Y4)**

Training users EPSC-DPS

# Future of data ingestion in SSHADE and its databases

## Starting databases:

- Start import published data
  - ➔ Aim to have **over 50 spectra by end of summer**

## Active databases:

- Check a few KW in your imported data (converted in v0.9.0), add some new option if needed
- continue to fill with Samples (+ Matters), Experiments & Spectra, Publications
  - ➔ focuses on published data (publication link)

SSHADE aim to have **over 2500 public spectra by end of summer (~ + 1000)**

## SSHADE common database (by SSHADE team)

- Check imported data (converted in v0.9.0)
  - ➔ continue to ingest **on request of the database managers (but we ask for help: prefill files)**
    - Fundamental Species & Phases and Objects, Bodies
    - some Reference Matters, Publications, Journals

# Discussion / Questions on database implementation

- Questions ??

# SSHADE Users

# Users outreach and training

## Past outreach / training sessions for users

At a few planetary and astrophysics conferences:

- European Lunar Symposium, May 2018, Toulouse, F
  - talk + 1 tutorial session
- EPSC sept 2018, Berlin, D
  - talk + 4 tutorial sessions
- DPS october 2018, Knoxville, US
  - at poster session

At a few national meeting, program and project meetings

In various reports : local, national ...

## Future user trainings:

- Pluto System After New Horizons, July 2019, Laurel, US
  - at poster session
- EPSC-DPS, sept 2019, Geneva, CH
  - with tutorial sessions and at poster session

Any other presentations of database(s) @ SSHADE by partners at other conferences ?

# SSHADE events Time line

## 2017

- December

**2nd SSHADE meeting**

## 2018

- January
- January
- March
- May-June-July
- August
- September
- October
- October
- December

8 active + 2 starting databases in SSHADE

**SSHADE infrastructure delivery**

**(D11.7 JRA VESPA)**

Training users ELS

Training database managers + SSHADE-Parties

11 active + 3 starting databases in SSHADE

**(D6.3 VAA VESPA – Y3)**

Training users EPSC

**(D6.5 VAA VESPA – Y3)**

Training database managers

Training users DPS

SSHADE-Party

## 2019

- May
- June
- July
- July
- August
- August
- September

**Major upgrade of SSHADE infrastructure and data (v0.9.0)**

**3rd SSHADE meeting**

Training users Pluto conference

≥ 18 active databases in SSHADE

**SSHADE with 18-20 databases**

**(D6.3 VAA VESPA – Y4)**

**End of Europlanet 2020-RI**

**(D6.5 VAA VESPA – Y4)**

Training users EPSC-DPS



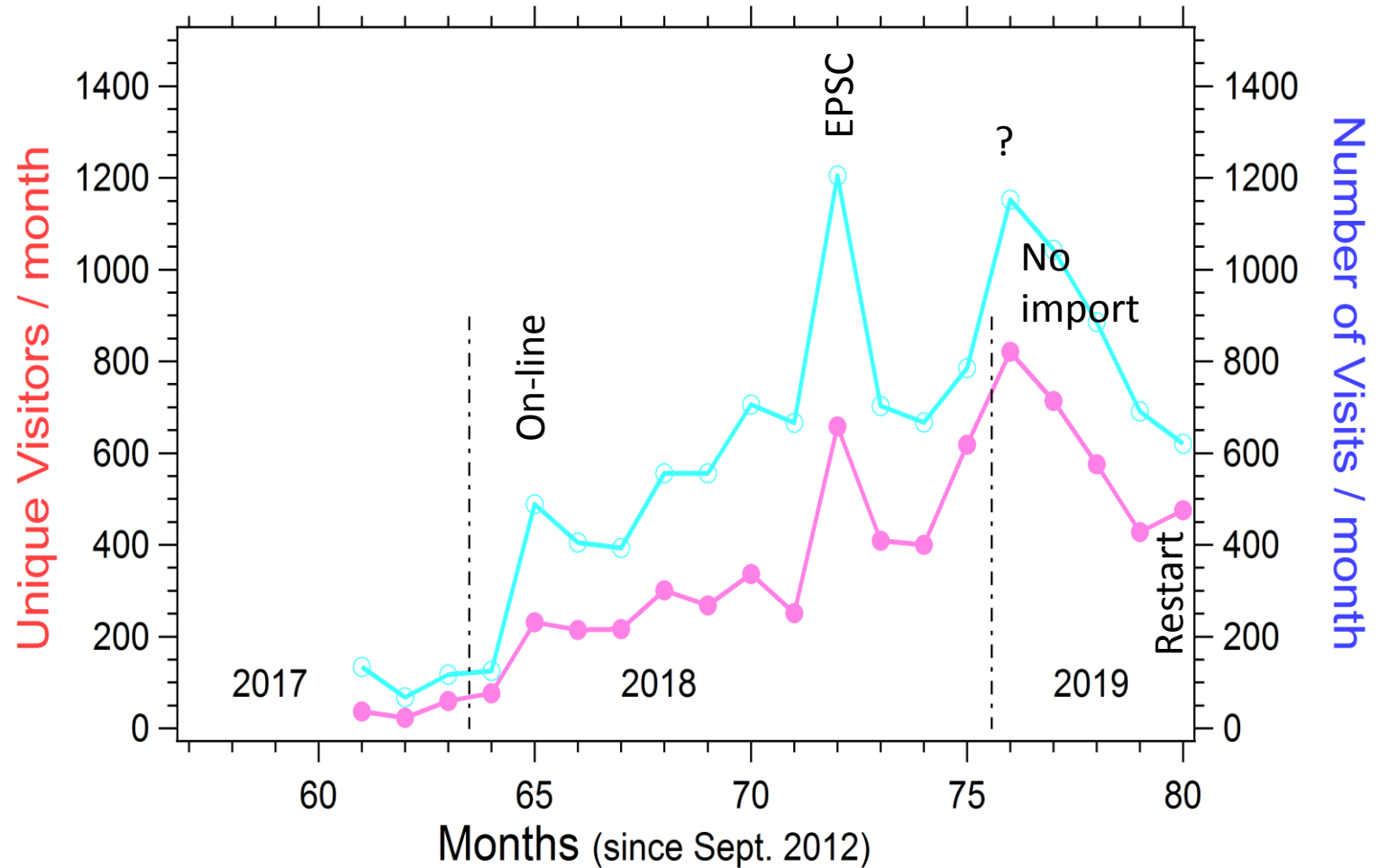
# SSHAE use Statistics

## Activity of users

2 tools: AwStats + Matomo

400-800 visitors / month

600-1200 visits / month



# SSHAE use Statistics

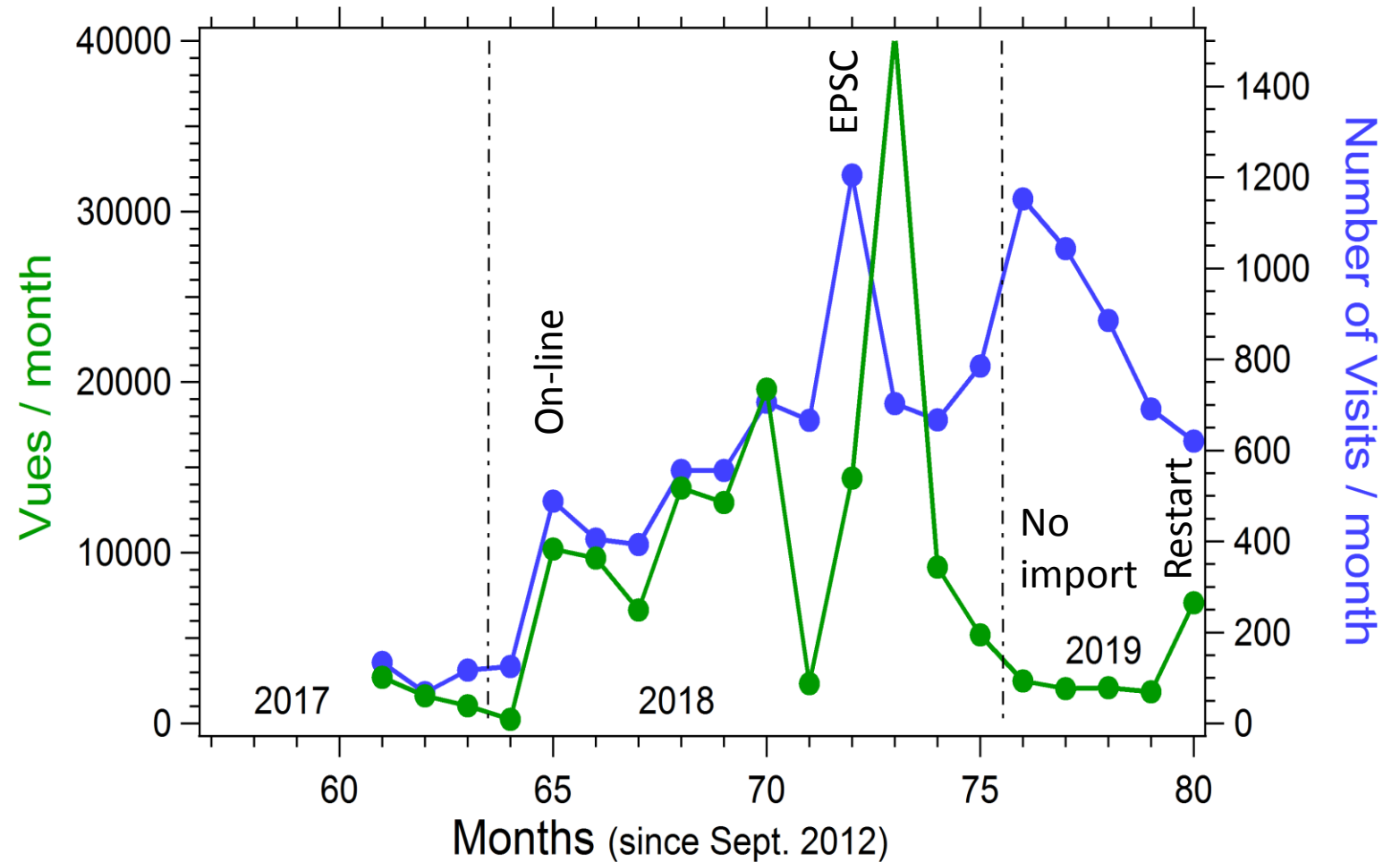
## Activity of users

2 tools: AwStats + Matomo

400-800 visitors / month

600-1200 visits / month

2000-20000 pages / month  
(Peak at 40000 ?!)



# SSHAE use Statistics

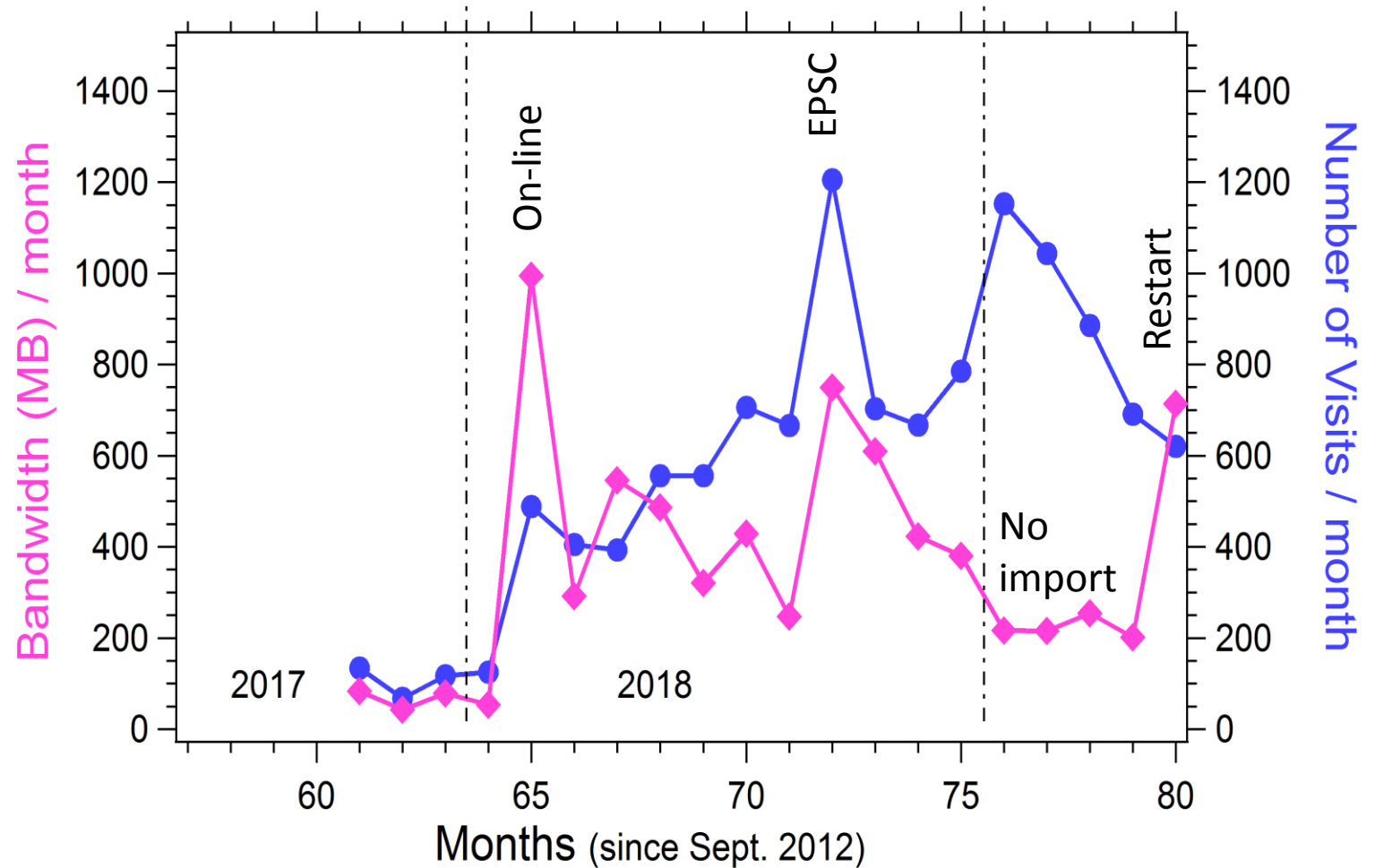
## Activity of users

2 tools: AwStats + Matomo

400-800 visitors / month

600-1200 visits / month

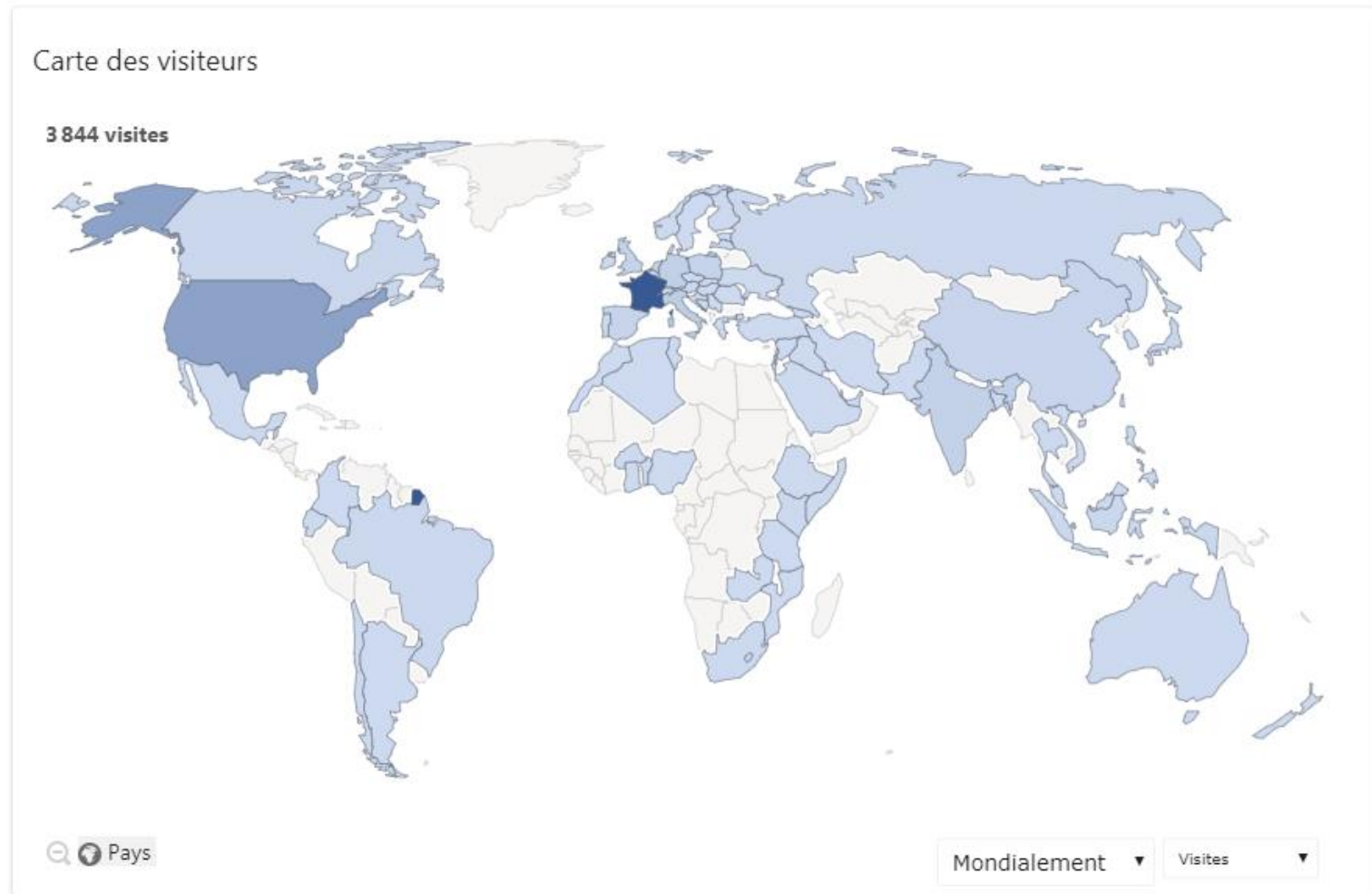
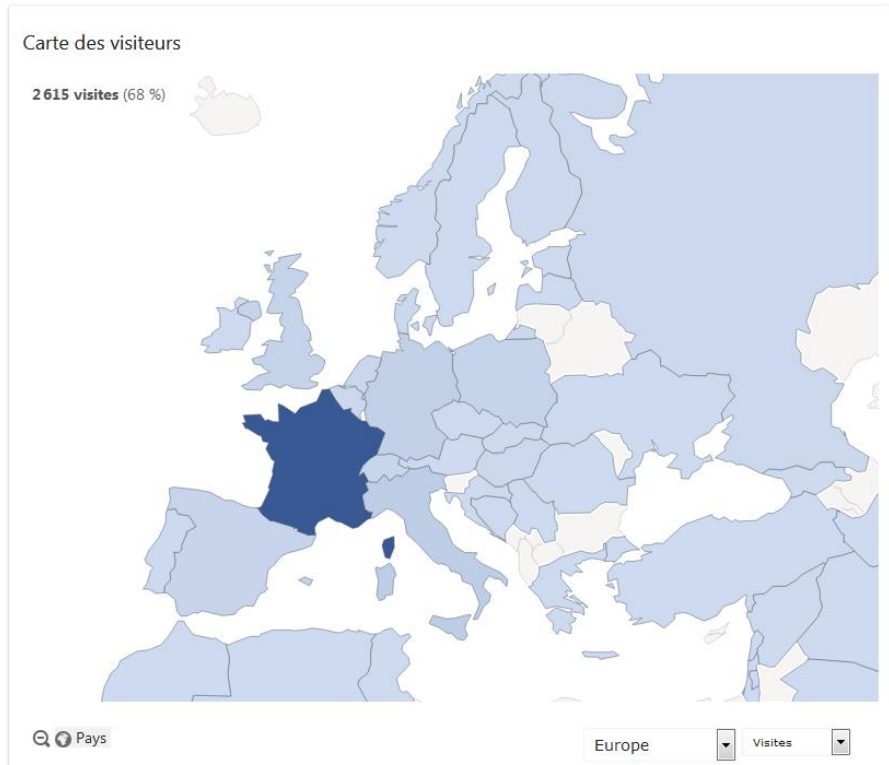
2000-20000 pages / month  
(Peak at 40000 ?!)



# SSHAE use Statistics

## Activity of users

### Map of the visits (2018-2019)



SSHADE advertising

# SSHADE advertising

## Advertise SSHADE by various ways

- Mail footers with web address
  - ➔ all SSHADE partners
- Newsletters
  - ✓ sent to 6 international astrophysics newsletters + 3 french newsletters
  - ➔ send to national newsletters
  - ➔ can be sent to other fields (geophysics, remote sensing, ...)
- Direct mailing
  - ✓ sent short 'advertisement' before EPSC 2018 to all participant who may use SSHADE data
    - => used the 1<sup>st</sup> author email in EPSC abstracts (~300), failed for DPS (no email available)
  - ➔ will redo for next EPSC-DPS 2019 (~1500 people) **[but need significant data content increase]**
  - ➔ **Mailing to other lists ?**

# SSHADE advertising

## Advertise SSHADE by various ways

- Conferences
  - ➔ SSHADE poster to post at all conferences  
=> will do one 'final' for EPSC 2019
  - ➔ Posters / talks on your database + SSHADE  
✓ at conferences, workshop, project meeting ...
  - ➔ Tell about / refer to SSHADE in your talks & posters, in your discussions, ...
  - ➔ distribute 'SSHADE visit card' at relevant posters
- Web Medias (FaceBook, Tweeter, ...) ? => TBD
- Other ideas ? ...

# SSHADE advertising : messages

## Some messages to communicate :

- SSHADE is not simply an interface for already existing databases (such as VAMDC, VOs, ...)
- SSHADE fosters the development of new databases and promote sof laboratory data
- SSHADE offers to the astronomers and Planetary scientist several types of experimental data to interpret their observations (by direct comparisons, modeling, ...)
- SSHADE is key for the exploitation of current and future space missions
- SSHADE is also key for the exploitation of current and future ground observatories
- SSHADE is much more than the 'test and calibration databases' of space instruments
- ...



SSHADE final infrastructure delivery

# Future SSHADE delivery to Europe

## To be delivered:

- SSHADE infrastructure 31st January 2018 (D11,8 JRA5 VESPA – Y1 & Y2)
- Filling of infrastructure + VO (D6.3 VA2 VESPA – Y3 & Y4)
- Training of providers and users (D6.5 VA2 VESPA – Y3 & Y4)

**Final delivery: 31st August 2019 SSHADE with 18-20 databases**

Less than 18 databases = failure *(we will assess this point beginning 2019)*

→ need to rapidly found other(s) *(we have a list...)*

## Documents to be delivered

- Delivery reports
- Documentation: manuals, tutorials, ...
- Blog, Wiki, ...

# State of data ingestion in SSHADE databases

Database	Matters	Samples	Experiments	Spectra
ACID		4	1	2
BYPASS	4	16	3	76
COMEDA		3	1	3
CSS		4	1	9
DAYSY	2	11	17	82
DOCCD	11	62	7	56
FAME	8	82	72	154
GhoSST	86	377	56	516
ISMAD		2	1	4
LSD	63	130	33	145
MIA	0	10	5	6
MTACSFK		1	1	1
PaSSTEL	15	12	13	18
REFL_SLAB		18	4	116

Database	Matters	Samples	Experiments	Spectra
RSPS		4	1	4
SCOOP		34	2	34
SOSYPOL	2	73	18	315
SPAN		15	5	20
SSTONE	6	370	7	370
STOPCODA	14	12	3	56
<b>Total</b>	<b>211</b>	<b>1270</b>	<b>251</b>	<b>1987</b>

## 20 Databases:

- 11 Actives
- 2 to be active
- 7 starting
- But the long 'import stop' for v0.9.0 upgrade is probably the main reason

# SSHADE infrastructure delivery to Europe (JRA 5)

## To be done before delivery:

- most databases: → provide a logo for your DB and upload using database.xml
- starting databases: → fill your database (after v0.9.0 tutorial)  
(ACID, COMEDA, CSS, ISMAD, MIA, MTACSFK, RSPS)

## Will be done soon (hopefully !):

- finalization + activation of the DOI

## You can do:

- Web page at your institution web site
  - start setting up a web page on SSHADE and your database
    - describing SSHADE (use text for SSHADE + logos, ... )
    - describing your database
    - with a link to SSHADE
    - tool for a 'first search windows' (that will redirect to SSHADE) will be provided later

SSHADDE in future Europlanet-2024 RI

# Euromplanet-2024 RI (2020-2023)

Budget: 10 M€

- Prepared : end 2018 – beginning 2019
- Submitted: March 2019
- Answer: summer 2019
- Start: February 2020
  
- **VESPA work package**
  - ✓ SSHADE but with a more limited budget  
(**< 2 years engineer**, **no support scientist** + much more limited travel budget)
  - SSHADE development: band list of molecular solids  
(+ extension of fundamental solids)
  - New partners => new databases (8 - 12)
  
- **TNA work package**
  - ✓ Continuation of TNA activity of CSS (spectro-gonio radiometers)
  - Bigger budget ...

# 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

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-pureCH4iceI-30K-NIR  
Original filename CH4-freq-tablel\_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

Showing 1 to 25 of 61 entries

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 / visualization /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 ? (→ 2020-21)

➔ need a permanent position

# SSDM fundamental solids extension ?

➔ for fundamental solid phases (molecular solids, ...)

- **Optical parameters**

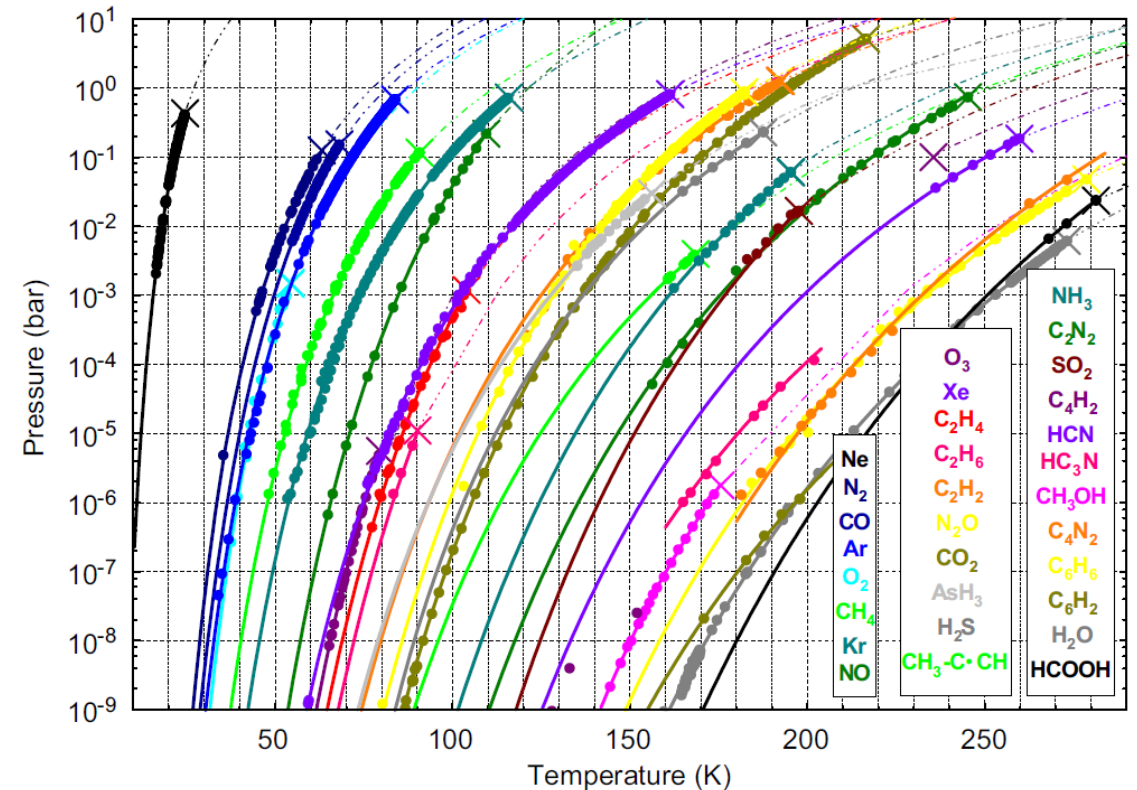
- optical indices
- birefringence
- ...
- Variation with temperature, pressure ...

- **Thermodynamic parameters**

- Vapor pressure
- Phase diagrams, ...
- Latent heat, heat capacity,
- Thermal conductivity, ...
- Variation of with temperature, pressure ...

- Publications + Partner's data

=> critical review and selection (partly done for  $P_S$ )



# New partners

## Future Databases:

In the frame of the current Europlanet proposal about 12 new partners will join the SSHADE infrastructure. The currently selected one are the following:

- University of Helsinki Astrophysical Scattering and Spectroscopy Laboratory, Univ. of Helsinki, FI 
- Planetary Sciences and Astrobiology, National Technical University of Athens, Athens, GR 
- Laboratório de Astroquímica e Astrobiologia, UNIVAP university, São Paulo, BR 
- Astrophysics Laboratory, University of Salento, Lecce, I 
- Planetary Science Institute School of Earth Sciences, China University of Geosciences, Wuhan, CN 
- Space Geodesy Group, Finnish Geospatial Research Institute, Masala, FI 
- Formation and Evolution of the Solar System and the Planets, CRPG, University of Lorraine, FR 
- a few additional partners will be selected during the first year of the Europlanet-2024 RI program.
  - ➔ New partner training,
  - ➔ 1-2 SSHADE meetings with current + new partners ?

SSHADE and databases sustainability

# SSHADE and databases sustainability

## Labelization of SSHADE infrastructure (+ French databases) by INSU/CNRS

4 December 2017

- => sustainability of infrastructure (by OSUG)
- => sustainability of French databases ...
- => some money from INSU (?), OSUG, other OSUs ?

## SSHADE development team employment in 2019-2020

- Damien Albert (development): permanent, part time
- Philippe Bollard (development): contract: full time => 09/2019 + part 2020 + ?
- Alexandre Garenne (support): ended 12/2018
- Lydie Bonal (support): permanent, part time (Astronomer service)

To guaranty SSHADE sustainability and development : **URGENT needs !**

- ➔ **Scientific support:** (Astronomer service) (scientific development/support): September 2020 ?
- ➔ **database/software engineer** position (development): 2020-2021 ?

# Tasks of SSHADE @ IPAG

## SSHADE infrastructure development

- SSDM (data model) for Bandlist + fundamental solids (?)
- Import tools for Bandlist, tools for users
- SSHADE interface improvements (visualization) + Band list
- VO interoperability (with VESPA, VAMDC, ...)

## Coordination of consortium

- Continue preparation of common fundamental data of SSHADE
- Development of the common 'band list database' (compilation, critical review...)

## Support to partners consortium

- Training of database managers + SSHADE party
- Completion of documentations and tutorials for providers
- On-line support

## Support to users

- Tutorials & training for users at conferences
- Preparation of documentations and tutorials
- By-mail support

# Tasks of the Scientific Managers and Database Managers

## Scientific manager

- define which data will be provided to the database
- scientific validation of data
  - ➔ responsible of the scientific content of its database
- animation of his data base
- contribution to the common « Band list » database

## Database manager

- prepare and test import files (all types)
- import data (sample, spectra, matters) + corrections
- report bugs, data errors and improvements
- Help in testing of infrastructure

# SSHADE and databases sustainability

up to end program and beyond ...

## SSHADE

- maintain/improve SSDM
- continue to improve the interface and tools
- need to keep active the users/providers access to the SSHADE infrastructure
- should ensure database partners training and support
- should ensure users training and support
- provide a repository for the data of the Europlanet TNA visits (spectroscopy)

## All databases

- need to keep 1-2 active Scientific/Database manager(s)
- continue to feed and maintain quality of their database
- animate their database + SSHADE (news, posters/presentation, ...), advertisements ...



# Summary of Managers actions

# Managers actions

## Active and starting databases

before final SSHADE report: (best before 30th july)

- Continue to ingest Samples, Experiments & Spectra, Publications
  - ➔ focuse on published data
- Put 'public' all data you can

For your SSHADE page:

Create a logo for your database

For Wiki

- Update the description of your database and its current content
- Description of typical sample / spectra type (only those already in SSHADE)
  - ➔ REFL\_SLAB, SCOOP, SPAN, ISMAD, MIA, MTACSFK, RSPS)
  - note: You can add a separate part describing future data you intend to put in SSHADE*
- Instruments, cells, techniques

# Managers actions

## Active and starting databases

- Provide the list of fundamental data (not yet present in SSHADE) you need in the coming months
- Report any error in SSHADE data (Fundamental species / phases / objects / Publication / ...) or in other databases
- Contribute to testing SSHADE user / provider interface => report at 'contact@sshade.eu'
- Create a Web page on SSHADE and your database at your institution web site
  - describing SSHADE (see text at SSHADE front page) + logos (SSHADE, Europlanet)
  - describing your database, with a link to SSHADE
  - tool for a 'first search windows' (that will redirect to SSHADE) will be provided later
- Provide a list the national and international newsletters you know + web link + contact

# Future reports and meeting

## Prepare contributions to deliveries and final report of VESPA VA

- Task 2. Enlarging content (beneficiaries) => SSHADE and database filling
  - Task 5. Dissemination & Sustainability => SSHADE and database sustainability
  - Task 6. Training => Users and SSHADE databases manager training
- 
- D6.10: 2<sup>nd</sup> set of standards documentation (month 46) => **June 2019**
    - ✓ SSDM v0.9.0
  - D6.14: 4th VESPA Annual report (month 48) => **July 2019**
    - ✓ DOI
    - ✓ EPN-TAP SSHADE
    - ✓ Partner databases content
  - Contribution to the final Europlanet report (month 48) => **July 2019**

# Logistics

# Logistics

- Monday we start at 10:30 and end at 6:00 pm
- Tuesday we start at 9:00 and end at 5:30 pm
- Wednesday we start at 10:00 and end at 5:00 pm
  
- lunches: will be taken at 'Camberra' restaurant at 12:30 (5 min from here)
  
- Dinner **Monday 3th 19:30 @ restaurant « Caffè Forté »**  
4 place de Lavalette  
Tram B stop : « Notre-Dame Musée »
  
- Dinner **Tuesday 4th 19:00 @ restaurant « L'Exception »**  
4 cours Jean Jaurès  
Tram B stop : « Alsace-Lorraine »

Dinner **Monday 3th**  
**19:30**

@ restaurant  
« **Caffè Forté** »

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06 07 62 25 05



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