



First SSHADE meeting – 16-17 Nov. 2020

SSHADE: Database Infrastructure of Solid Spectroscopy



<https://www.sshade.eu>

Bernard Schmitt, Philippe Bollard, Damien Albert, Manon Furrer,
Lydie Bonal, Olivier Poch and the SSHADE Consortium Partners

EUROPLANET 2024-RI - VESPA VA2

Aims of this 1st SSHADE partner's meeting

To present:

- the project and the tasks to be realized during the 4 years of the Europlanet 2024-RI program.
- the current state and plans of development of :
 - the SSHADE database infrastructure
 - the Band List database
 - the Partner's databases

To discuss:

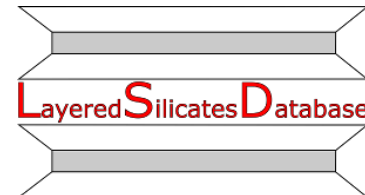
- about organization of database managers training sessions
- any question related to SSHADE



The SSHADE database infrastructure

for Astrophysics, Planetary sciences and Geosciences

- ✓ **Promote** the creation of databases of laboratory & field **spectra of solids** in the **electromagnetic spectrum**
- ✓ **Develop** tools & interface to provide on-line the experimental data
 - ✓ **Develop** tools to analyze and use the data
- ➔ Host a set of databases from a Consortium of research groups



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

Main aim of *SSHADE*

- **Provide to the planetary and astrophysics community**

- **Spectral and spectro-photometric data**

- on all types of solid materials (but also liquid)
- from synthetic, terrestrial or extraterrestrial samples

- **with well documented information !!**

- on the spectra, samples, experiments ... + publications

- **with a data reference and a DOI per experiment**

- easy to cite & provides direct access to the data used

→ **For the analysis, modeling and interpretation of spectroscopic observations**

of planetary surfaces, aerosols & grains, + inter- & circumstellar grains, exoplanets...

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**
- 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 Europlanet-2020 RI (VESPA JRA)
Opening of SSHADE to participating European (+Indian) partners (VESPA VA)**
- ✓ **1 Feb. 2018: SSHADE online with 10 databases (1250 spectra)**
- **Nov. 2020: SSHADE with 17 active databases (> 3700 spectra)**
- ✓ **2020-2023** **Europlanet-2024 RI : development of ‘band list of solids’ database (prototype: August 2021)
Addition of 10-12 databases from around the world**

Solid Spectroscopy database Infrastructure

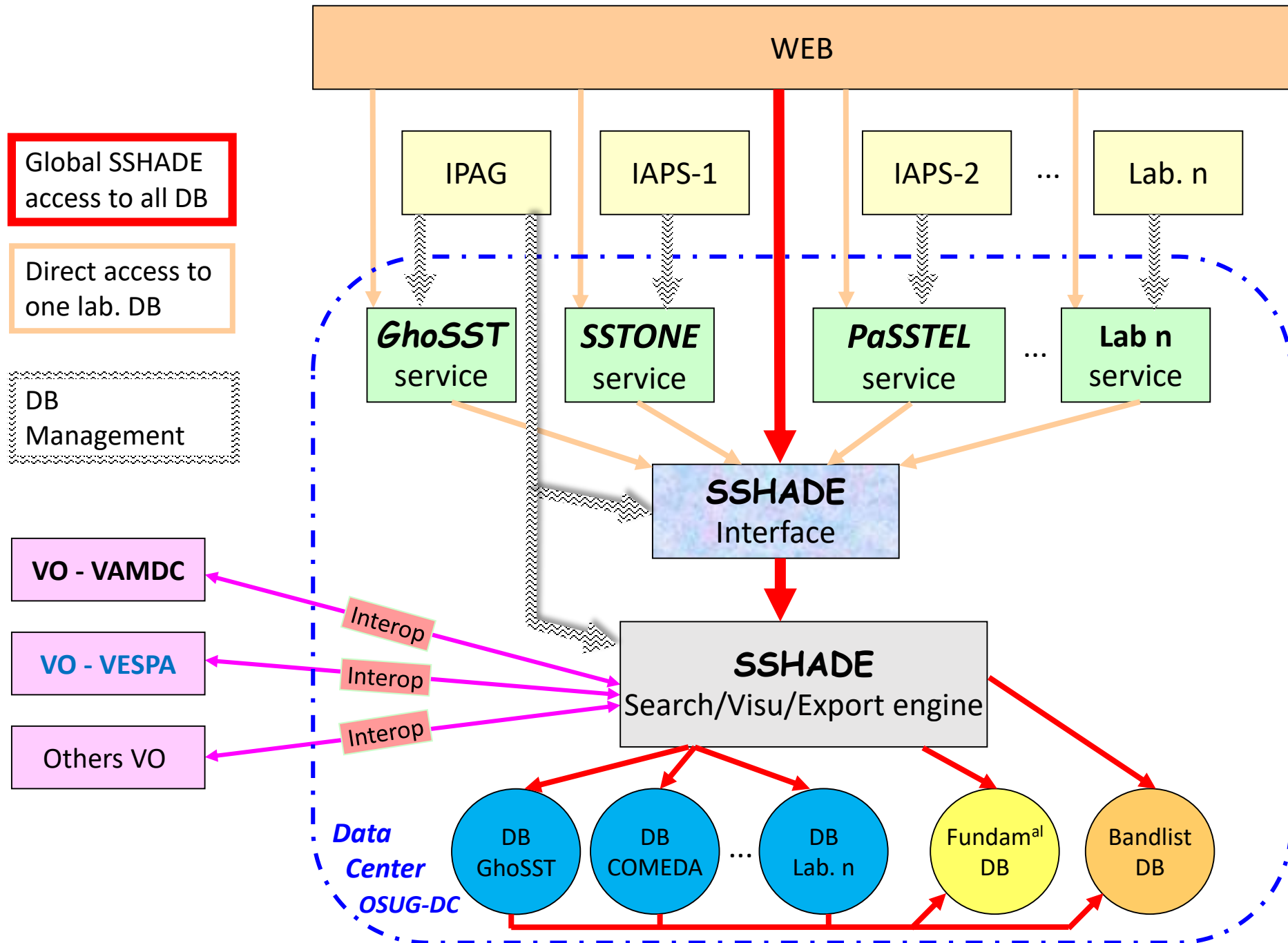
SSHADE

“Solid Spectroscopy Hosting Architecture of Databases and Expertise”

- Based on the *Solid Spectroscopy Data Model (SSDM)*

Made of:

- ✓ an interface specialized in ‘solid spectroscopy’
 - ✓ an Import / Search / Visualization / Export engine
 - ✓ a common fundamental database
 - ✓ a set of databases: one per partner / group
- All hosted at OSUG data center (OSU Grenoble – UGA)
 - SSHADE is a service of others VO (VESPA-VO, VAMDC, ...)



SSHADe Consortium of Data Providers

Data from **20 solid spectroscopy experimental groups** in **10 countries** (~70 researchers)

New (2020-2023) : **10-15** new groups (7+ new countries) (~60 researchers)

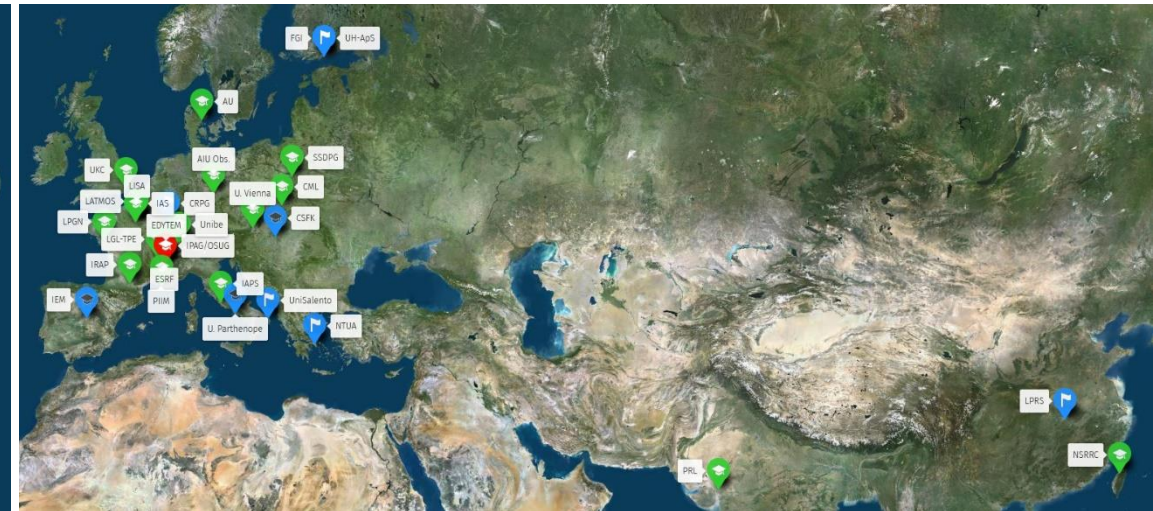
17 active databases + **3 starting** + **10-12 coming**

Each with particular expertise on:

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

SSHADe : www.sshade.eu

SSHADe Wiki : wiki.sshade.eu



17 active databases* + 4 starting

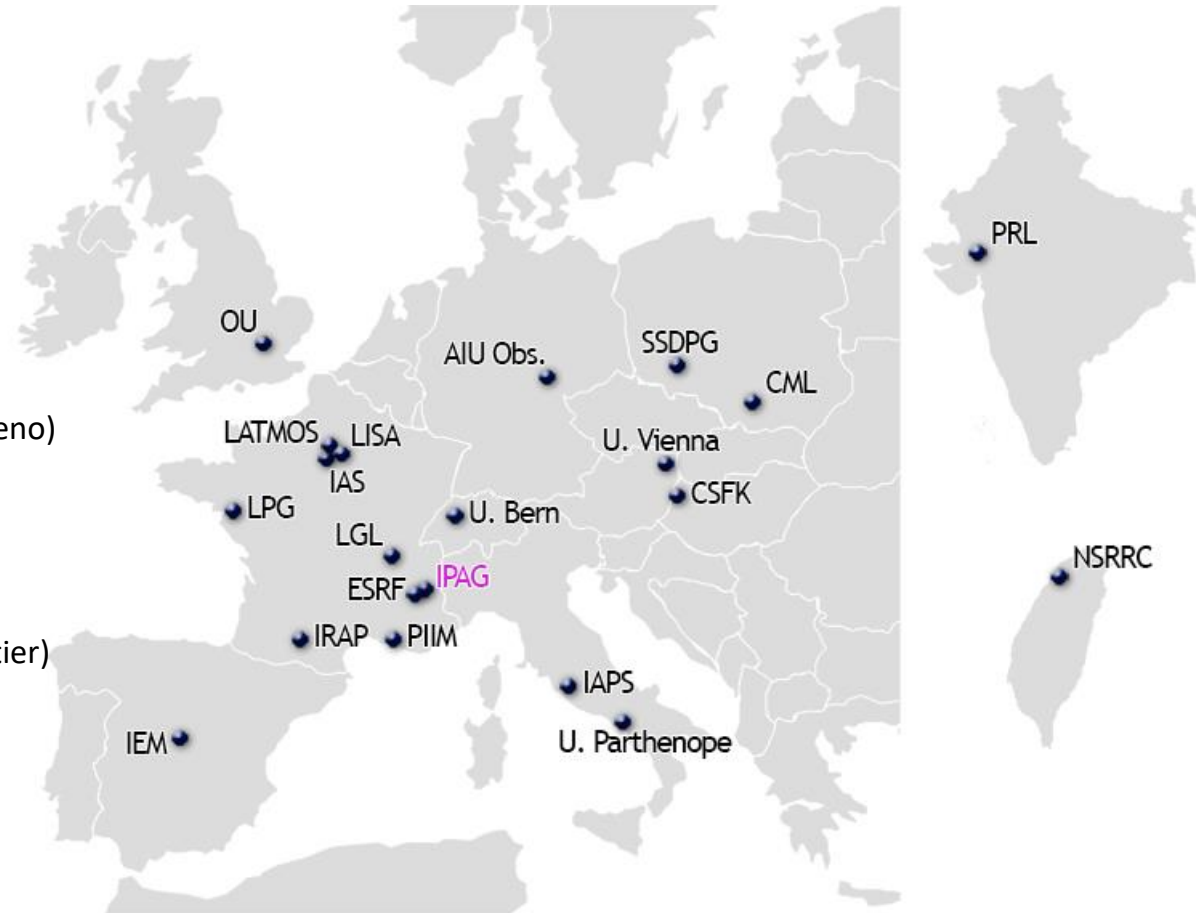
Hosted databases

 ACID 25 spectra	 BYPASS 123 spectra	 COMEDA 3 spectra	 CSS 276 spectra	 DAYS 82 spectra	 DOCCD 127 spectra
 FAME 396 spectra	 GhoSST * 1186 spectra	 ISMAD 4 spectra	 LSD 146 spectra	 MIA 6 spectra	 Mirabelle 2 spectra
 MTACSFK 1 spectrum	 PaSSTEL 24 spectra	 PIG 45 spectra	 REAP 41 spectra	 REFL_SLAB 158 spectra	 SCOOP 34 spectra
 SOSYPOL 278 spectra	 SPAN 20 spectra	 SSTONE 370 spectra	 STOPCODA 56 spectra		

The SSHADE-Europe consortium in EPN@2020-RI

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

- **IPAG / Planéto**, 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)
- **LATMOS / IMPEC**, Institut Pierre Simon Laplace - F (Nathalie Carrasco, Thomas Gautier)
- **IAPS**, INAF, Roma - I (Alessandra Rotundi, Andrea Longobardo)
- **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)
- **National Synchrotron Radiation Research Center (NSRRC)** - Hsinchu City, TW



SSHADE : The team

Scientific team

- Bernard Schmitt (SSHADE Manager)
- Lydie Bonal
- Olivier Poch

Development team :

- Philippe Bollard (technical manager, developer, leaving very soon)
- Damien Albert (developer, part time)
- Manon Furrer (developer, full time since sept. 2020)

For each databases:

- Scientific manager
- Database manager
- Data providers

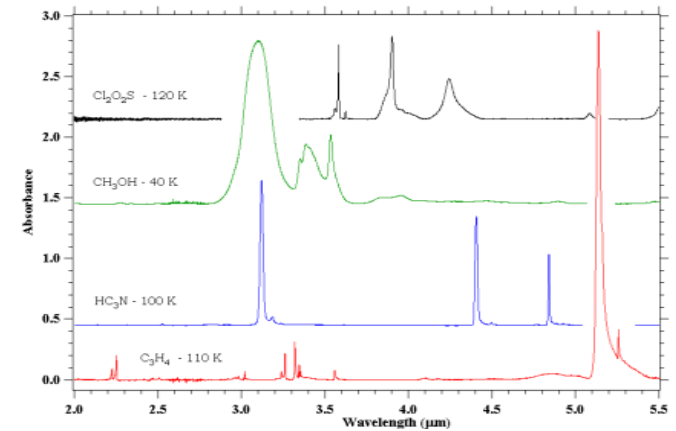
Which types of materials and samples in *SSHADE* ?

• Materials

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

• Samples

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



Which types of spectra in *SSHADE* ?

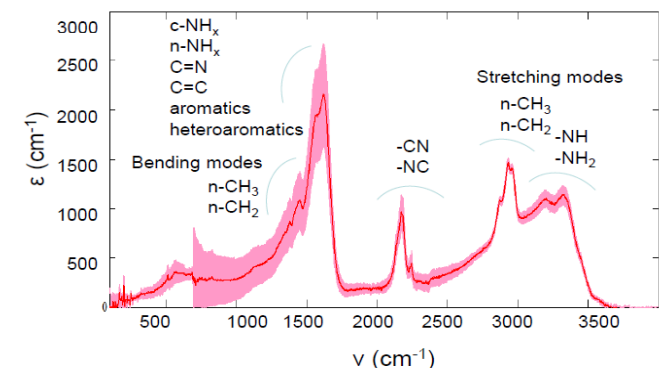
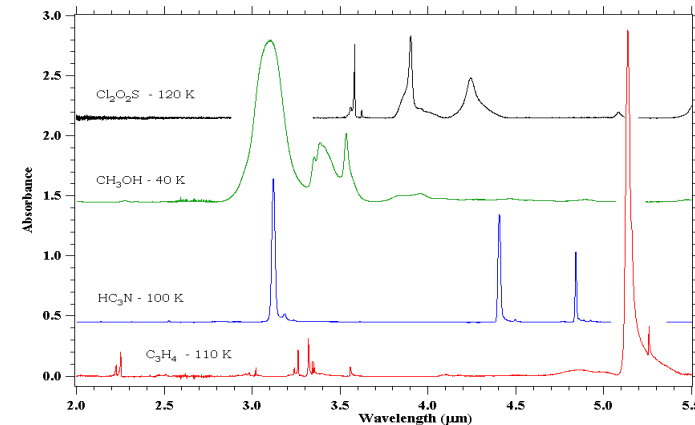
- **Spectral ranges:**

- Designed from γ -rays to radio wavelengths
- Now mostly from **VUV to sub-mm (0.2 μm - 1mm)**, plus **X-rays**.

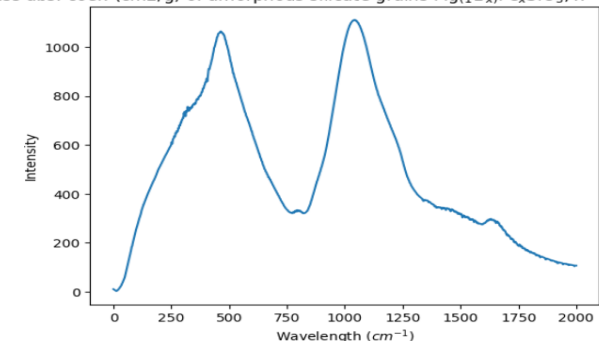
- **Types of data:** (from level 1 to 5)

- **Spectra**

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



Mass abs. coef. (cm^2/g) of amorphous silicate grains $\text{Mg}_{(1-x)}\text{Fe}_x\text{SiO}_3$, $x=0.0$ to 1.0



Types of data for Planetary surfaces

- **Laboratory data:**

- **Optical constants of ices** => radiative transfer
- **Reflectance** spectra of mineral, salts, organic & icy surfaces
 - Effect of grain size
 - Effect of temperature (90 – 500 K)
 - Effect of adsorption of H₂O
 - Effect of high pressure
- **Spectro-photometric functions** of mineral and icy surfaces
- **Raman** spectra & micro-spectroscopy of minerals
- **Surface processes:** differential sublimation of ices, space weathering, ...
- ...

- **Planetary data:**

- **Reflectance** spectra of Moon soils, ...
- **Reflectance, Raman** spectra of Meteorites, IDPs, ...

VNIR reflectance spectra of Thermanatrite with 3 different grain sizes and at variable temperature (93-279 K)

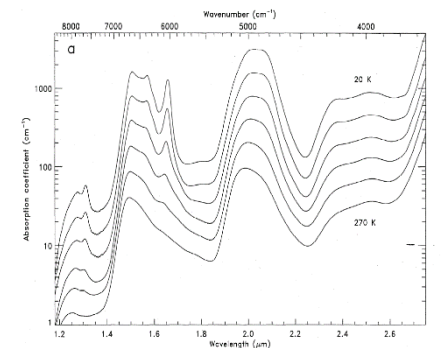
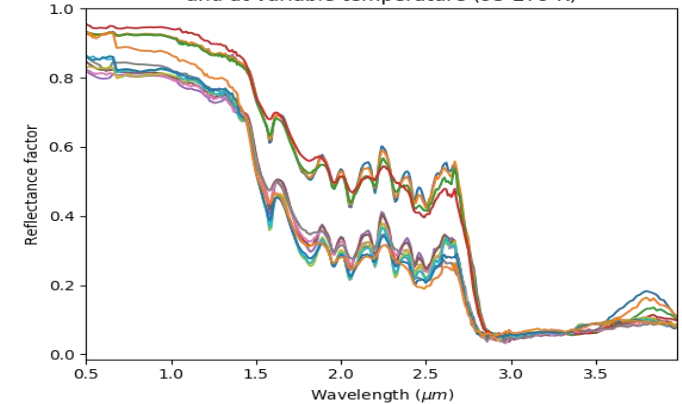


Figure 2. Illustration of the temperature dependence of our H₂O ice absorption coefficients. (a)

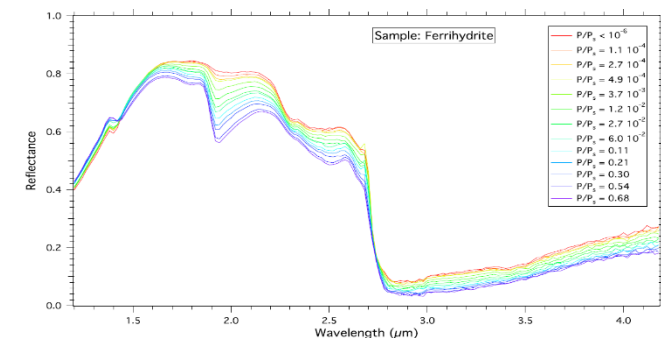


Fig. 11. Reflectance spectra of the ferrihydrite sample measured under different values of water vapor relative pressure.

Questions on SSHADE (content, ...)

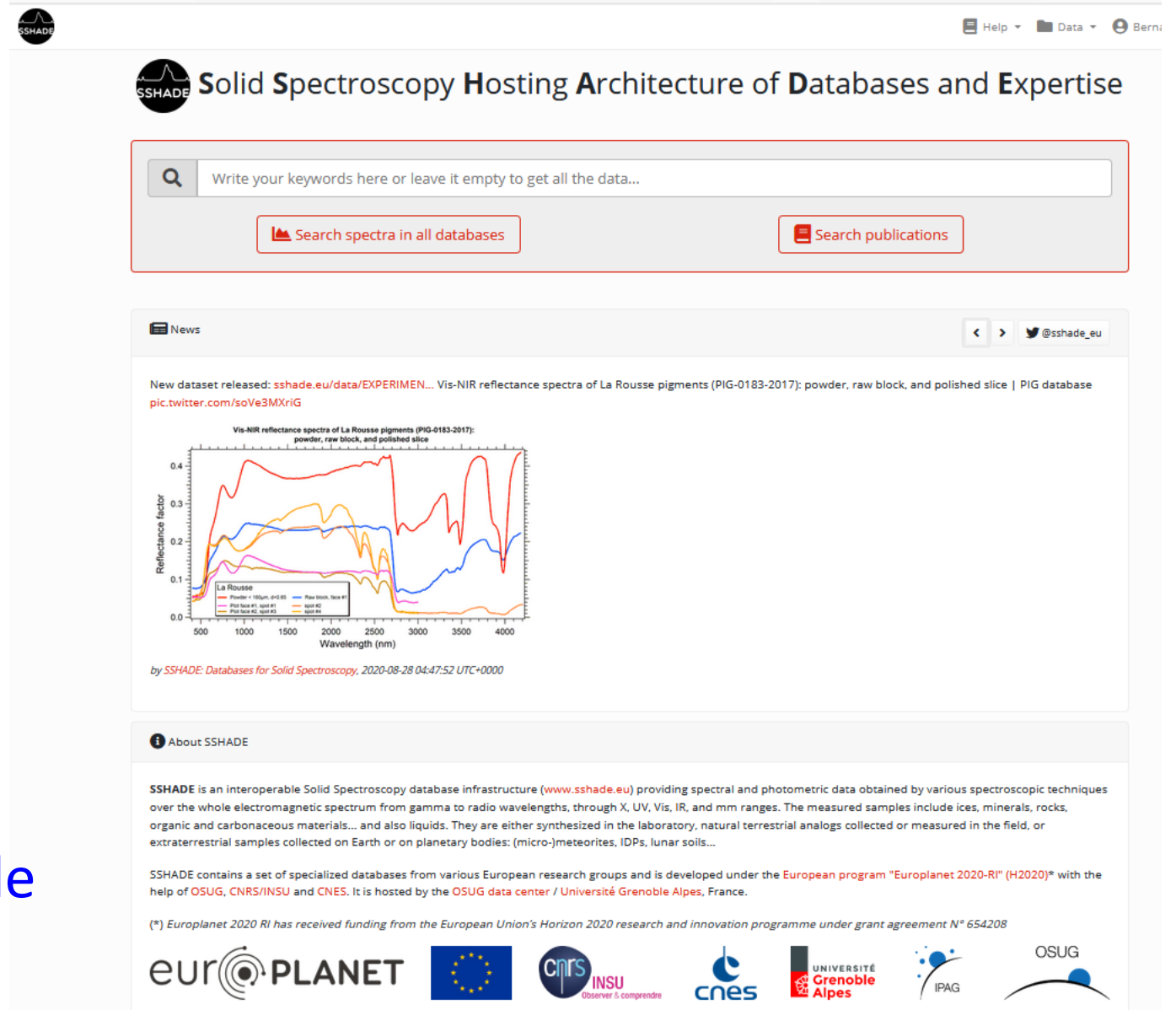
SSHADÉ : user interface

www.sshade.eu

Search bar →

News and new data →

Already over 3400 spectra available
(+ ~300 in preparation)



The screenshot displays the SSHADÉ website interface. At the top, the title "Solid Spectroscopy Hosting Architecture of Databases and Expertise" is visible. A search bar is present with the placeholder text "Write your keywords here or leave it empty to get all the data...". Below the search bar are two buttons: "Search spectra in all databases" and "Search publications".

The "News" section features a "New dataset released" announcement for "sshade.eu/data/EXPERIMEN... Vis-NIR reflectance spectra of La Rousse pigments (PIG-0183-2017): powder, raw block, and polished slice | PIG database". Below this is a line graph titled "Vis-NIR reflectance spectra of La Rousse pigments (PIG-0183-2017): powder, raw block, and polished slice". The graph plots "Reflectance factor" (y-axis, 0.0 to 0.4) against "Wavelength (nm)" (x-axis, 500 to 4000). The legend indicates: "La Rousse", "Powder - 100µm, 400-600", "Raw block, face #1", "Powder face #1, 400-600", "Powder face #1, 600-800", "Raw block, face #1", "Powder face #1, 800-1000", and "Powder face #1, 1000-1500".

The "About SSHADÉ" section describes the project as an interoperable Solid Spectroscopy database infrastructure providing spectral and photometric data. It mentions that the data is developed under the European program "Europlanet 2020-RI" (H2020)* with the help of OSUG, CNRS/INSU, and CNES. It is hosted by the OSUG data center / Université Grenoble Alpes, France.

Footnote: (* Europlanet 2020 RI has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement N° 654208)

Logos for eur@PLANET, the European Union, CNRS INSU (Observer & comprendre), CNES, Université Grenoble Alpes, IPAG, and OSUG are shown at the bottom.

User interface

- **Search tool + results**

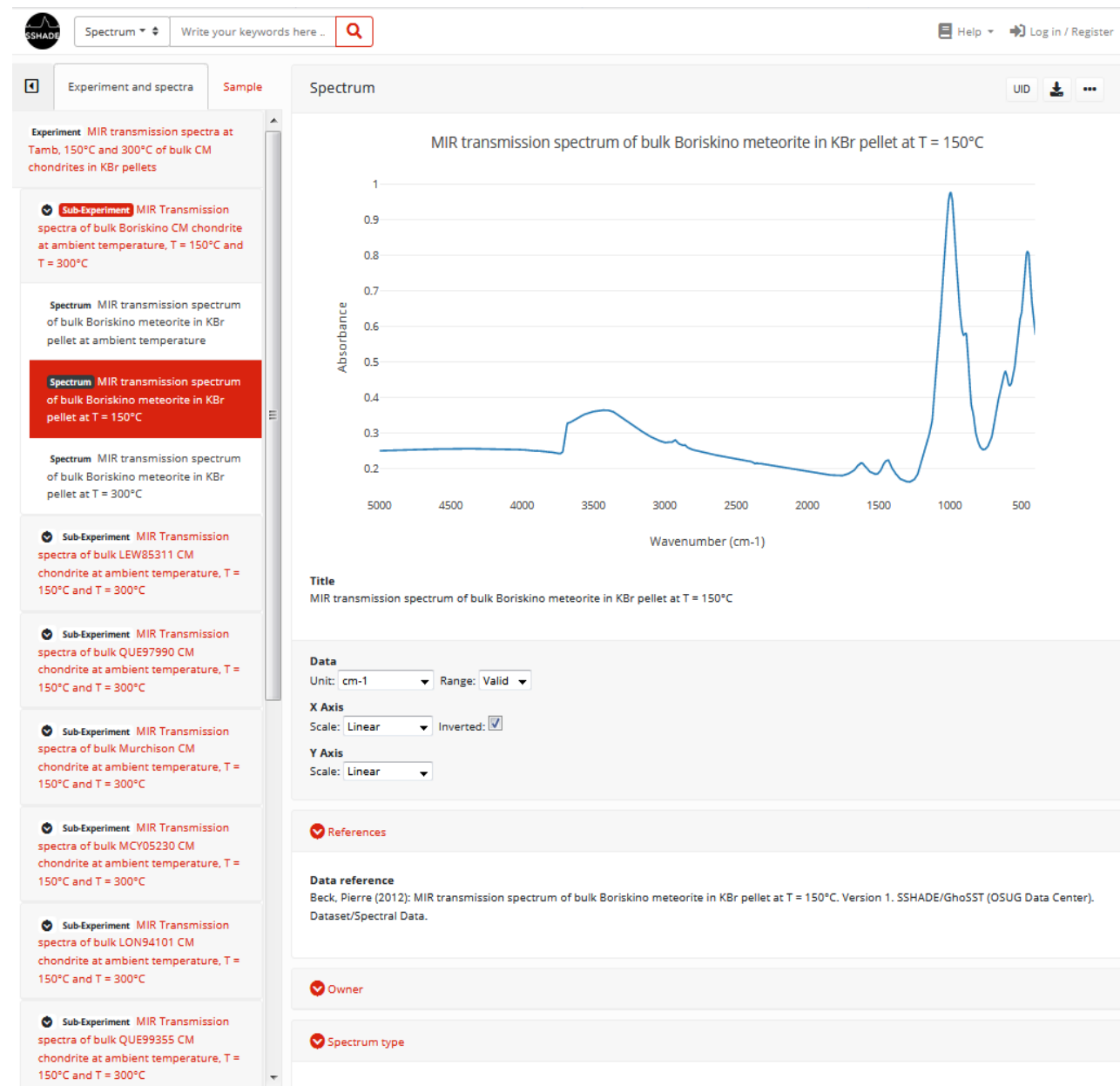
- ✓ Spectra
- ✓ Publications
- ✓ **Bandlist**

- **Data display :**

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

- **Export :**

- Experiment, Spectra, sample details
- w. links to associated information
- Custom export (unit, range, format ...)
- Dashboard (export history, ...)



SSHADE Wiki

<https://wiki.sshade.eu>

SSHADE infos

SSHADE fact sheet

SSHADE databases

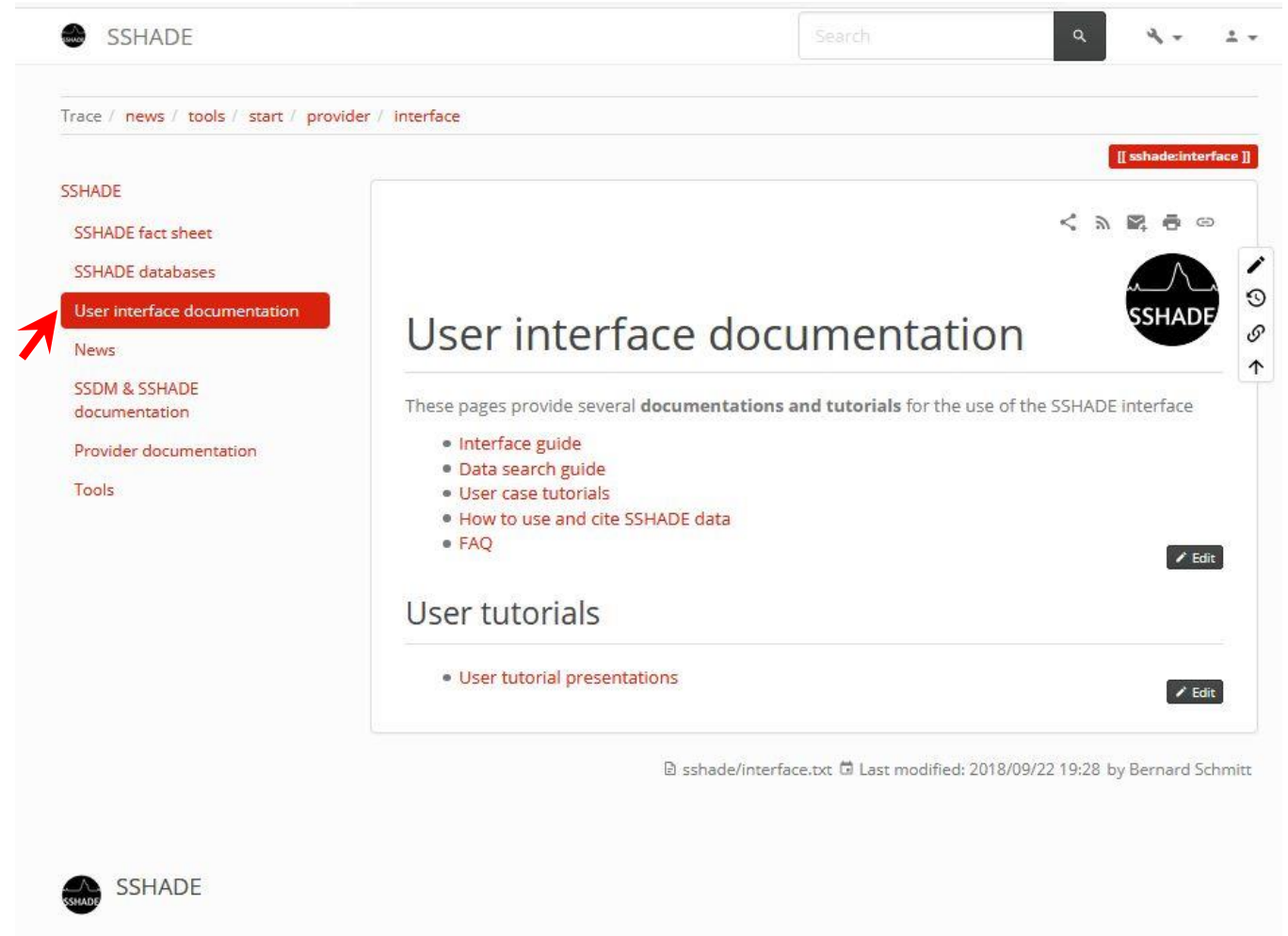
User help (interface documentation)

News

SSDM & SSHADE documentation

Provider documentation

Tools



The screenshot shows the SSHADE Wiki page for "User interface documentation". The page title is "User interface documentation" and it includes a list of links for "Interface guide", "Data search guide", "User case tutorials", "How to use and cite SSHADE data", and "FAQ". The page also features a "User tutorials" section with a link for "User tutorial presentations". The page is edited by Bernard Schmitt on 2018/09/22 19:28. The SSHADE logo is visible in the top right and bottom left corners.

Trace / news / tools / start / provider / interface

[[sshade:interface]]

SSHADE

SSHADE fact sheet

SSHADE databases

User interface documentation

News

SSDM & SSHADE documentation

Provider documentation

Tools

User interface documentation

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

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

User tutorials

- User tutorial presentations

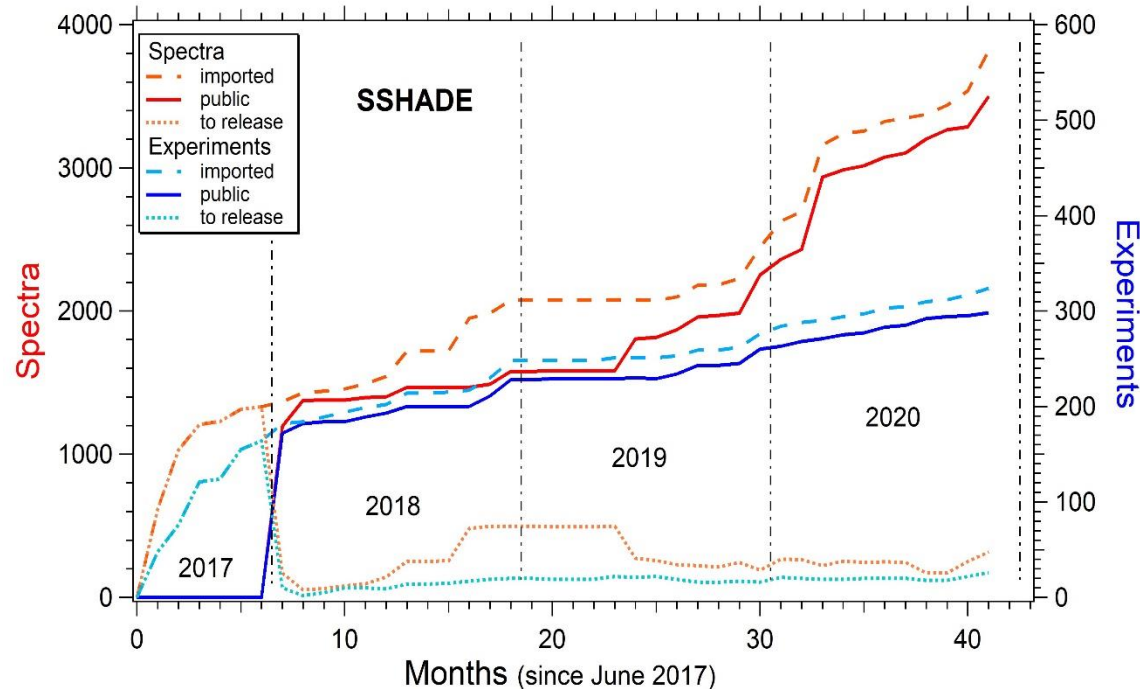
sshade/interface.txt Last modified: 2018/09/22 19:28 by Bernard Schmitt

The users of SSHADE

Increase of content and of use

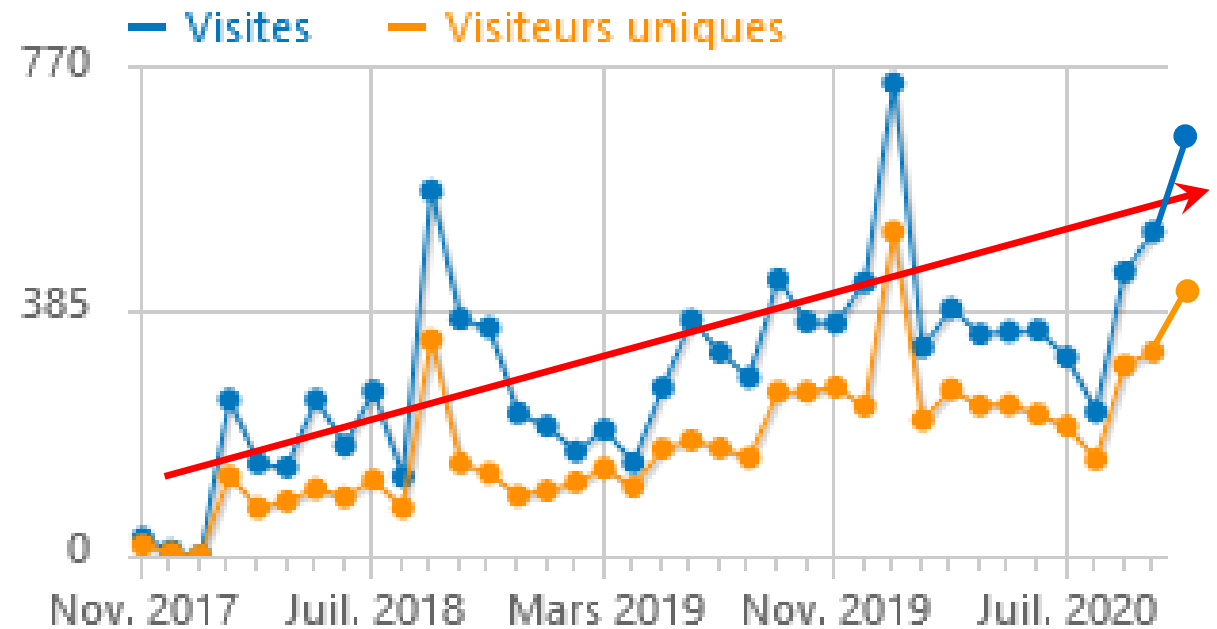
- Over 220 researchers registered
- SSHADE data content

Experiments & Spectra



SSHADE visits (Stats Matomo)

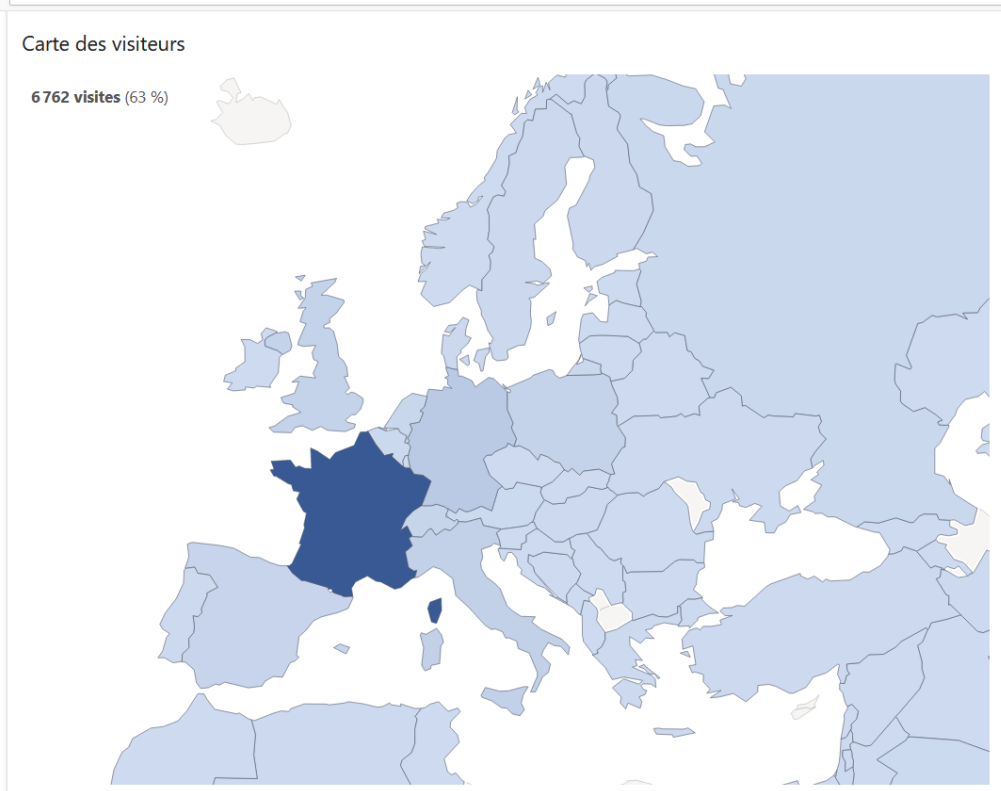
40% France, 20% Europe, 20% USA+Canada, 17% Asia



SSHAE use Statistics

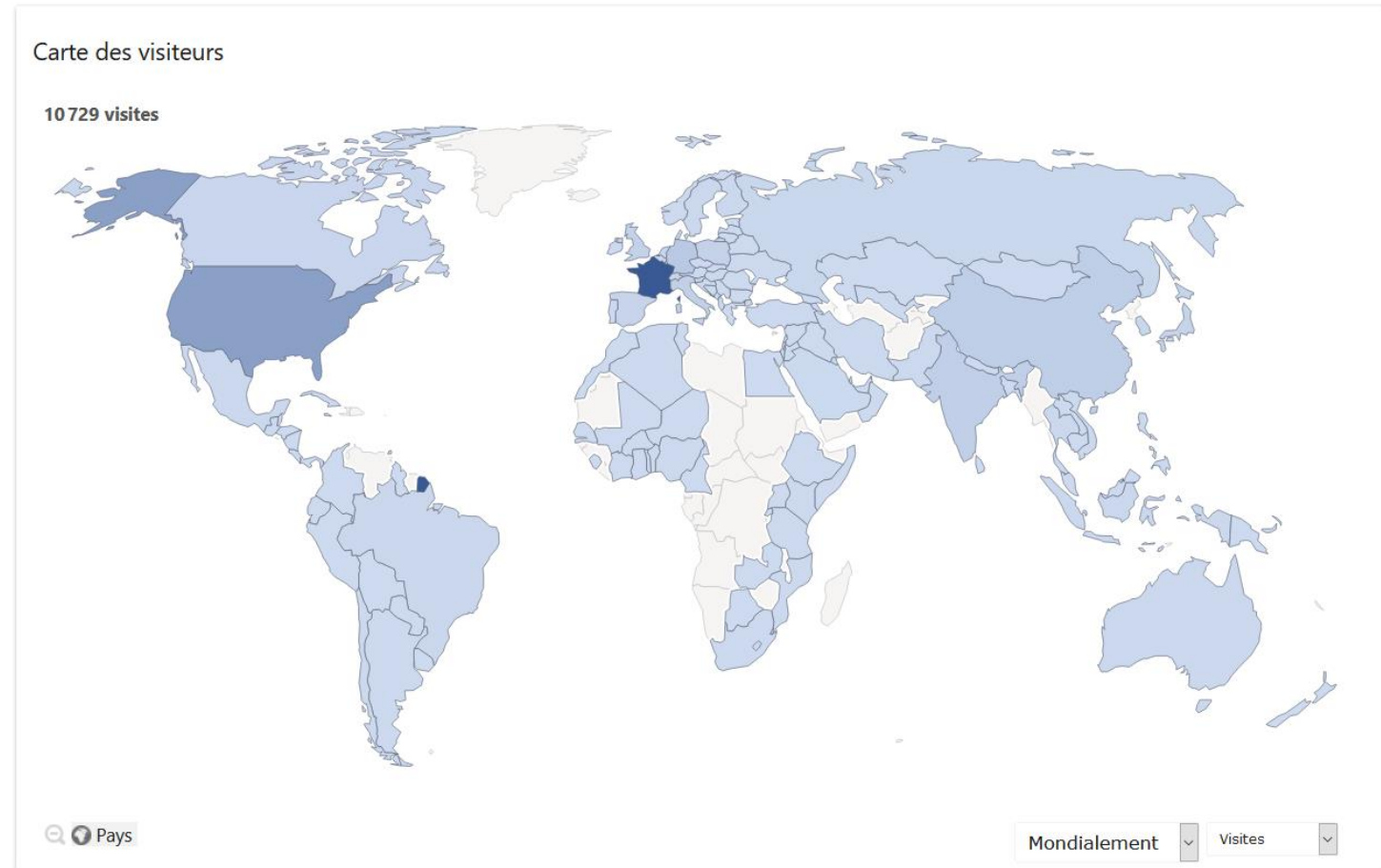
Activity of users

Map of the visits (2018-2020)



SSHAE visits (Stats Matomo)

40% France, 20% Europe, 20% USA+Canada, 17% Asia



Behind the scene

- **The development team**
- **The Solid Spectroscopy Data Model**
- **The fundamental data**
- **The links with the Virtual Observatories**

Who do what ?

SSHADE management

- *Scientific Manager:* Bernard Schmitt
- *Software Manager:* Philippe Bollard => ?? (summer 2012)

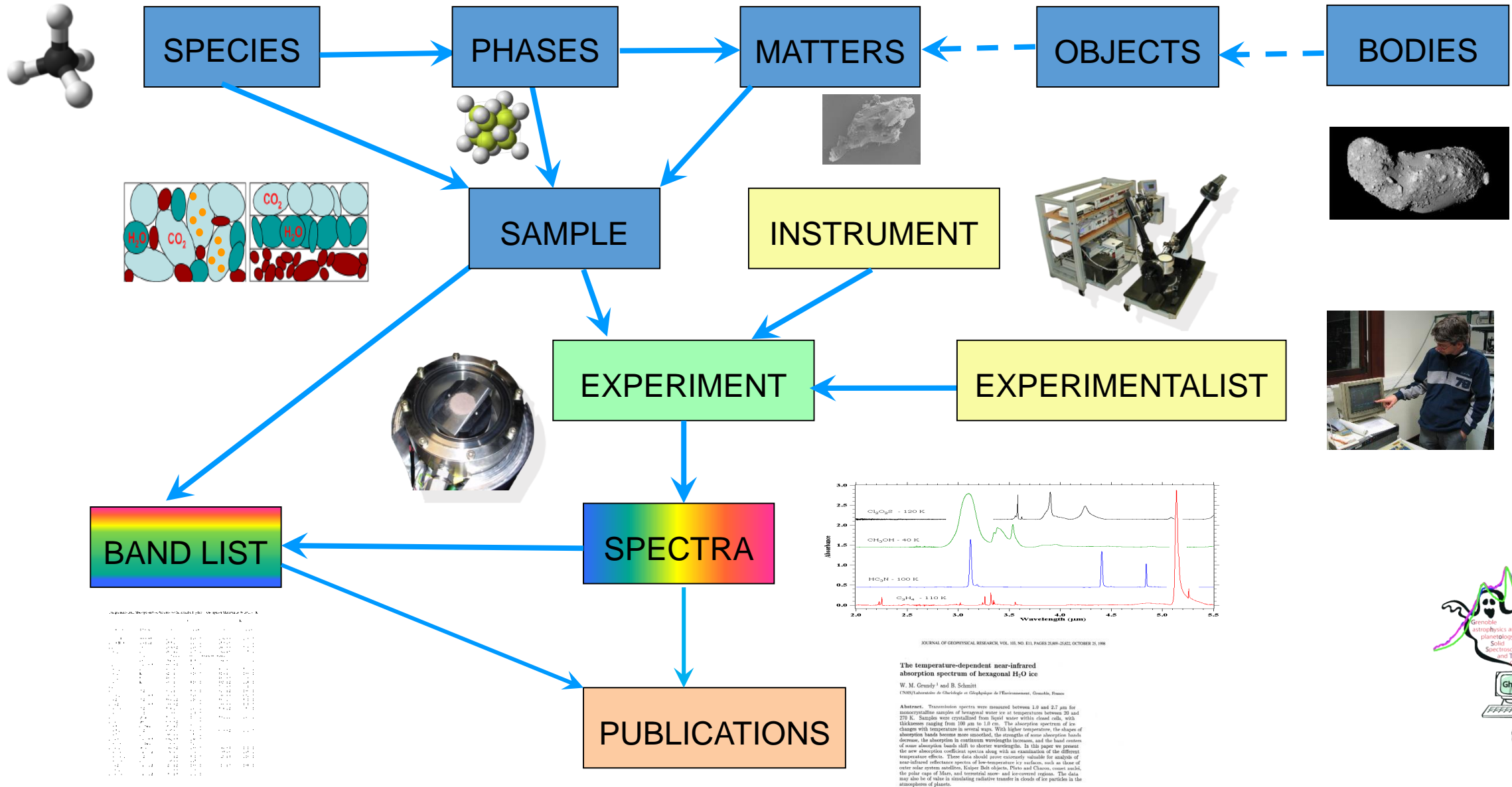
SSHADE development

- *Datamodel development* Bernard Schmitt + LB + OP
- *Databases development:* Philippe Bollard, Damien Albert
- *Band list database dev.:* Manon Furrer
- *VO interoperability:* Damien Albert

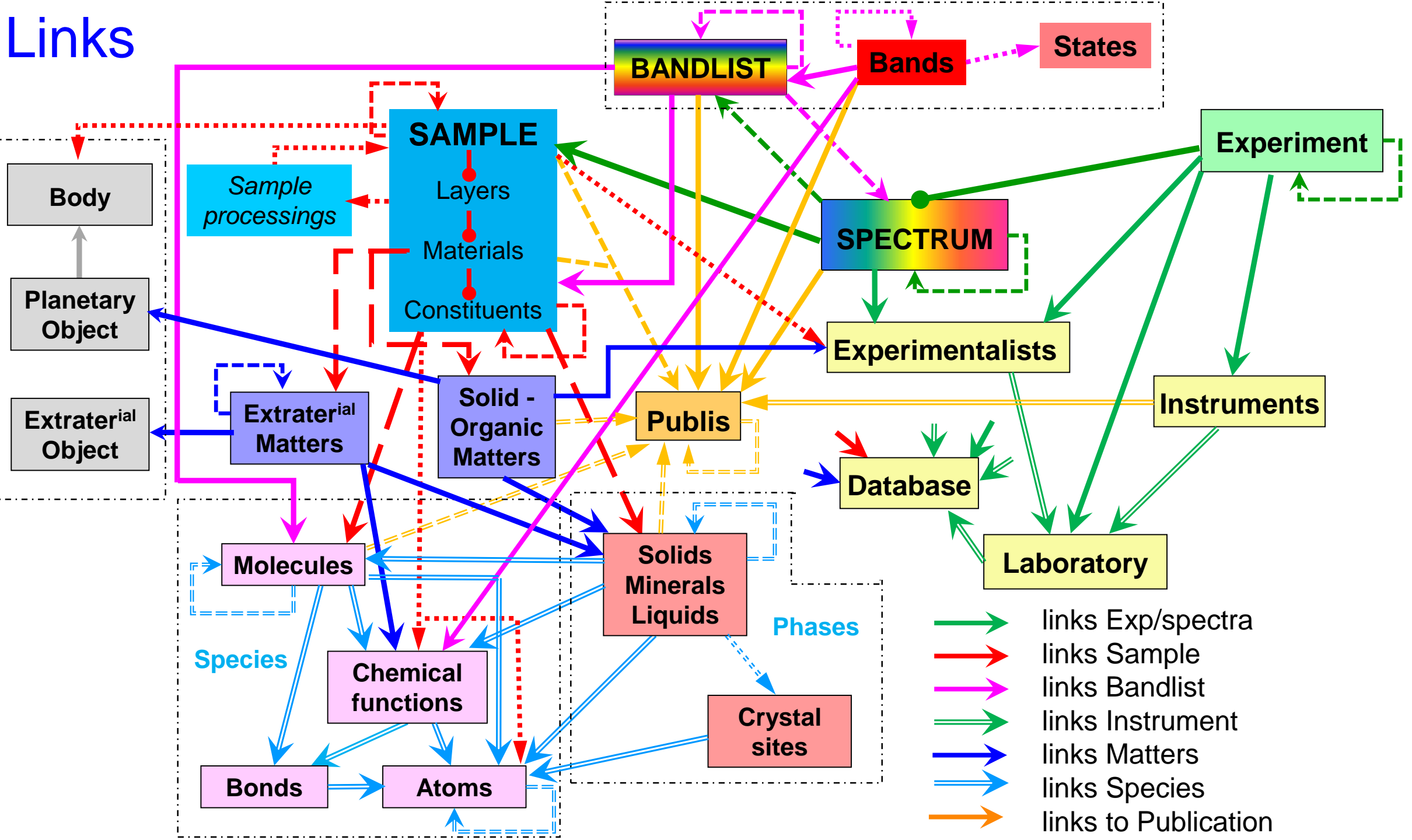
Data bases feeding

- *Consortium/users support:* Bernard Schmitt + LB
- *Fundamental data feeding* Lydie Bonal + Olivier Poch + BS
- *Data validation, DB animation* Scientific Managers (one at each consortium group)
- *Data preparation & import* Database Managers (one at each consortium group)

The Solid Spectroscopy Data Model - General Structure



Links



Fundamental Data feeding:

For SSHADE 'Public'

May 2016

Nov. 2020

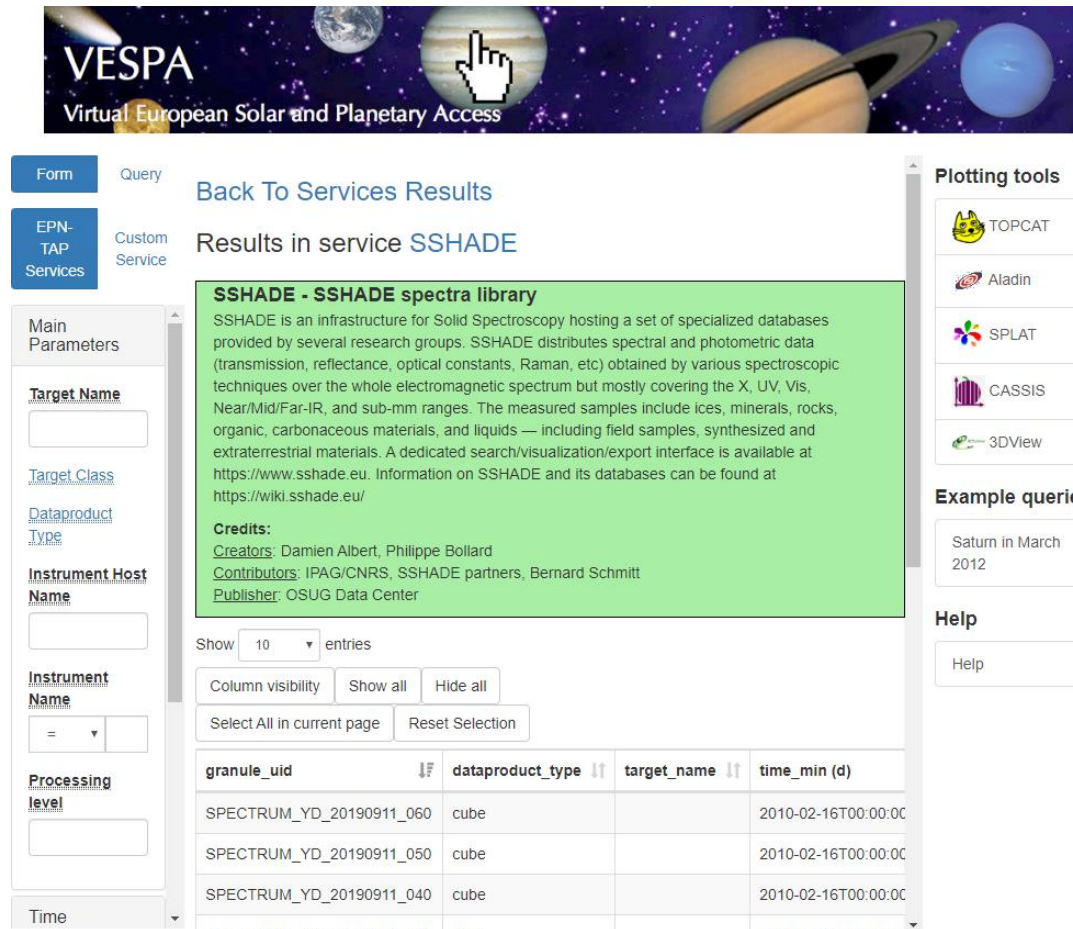
• Species:		
• Atoms/ Chem Fct	→ 120 /276	185 /392
• Molecules	→ 85	195
• Minerals	→ 104	237
• Solids / liquids	→ 12 / 2	191 / 10
• Meteorite objects	→ 78	187
• Micrometeorite / IDPs	→ 0	11 / 5
• Band lists / bands		
• Molecular solids + adsorption	--	1 / 30
• Publications	→ 125	320

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)

→ public VO completed and delivered in summer 2019



The screenshot displays the VESPA interface. At the top is a banner with the text "VESPA Virtual European Solar and Planetary Access" and a hand cursor pointing to a planet. Below the banner are navigation tabs for "Form", "Query", "EPN-TAP Services", and "Custom Service". The main content area shows "Back To Services Results" and "Results in service SSHADE". A green box highlights the "SSHADE - SSHADE spectra library" description, which states that SSHADE is an infrastructure for Solid Spectroscopy hosting specialized databases. Below this is a table of search results with columns for granule_uid, dataproduct_type, target_name, and time_min (d). The table lists three entries for SPECTRUM_YD_20190911_060, 050, and 040, all of type 'cube' and with a time_min of 2010-02-16T00:00:00. On the right side, there are sections for "Plotting tools" (TOPCAT, Aladin, SPLAT, CASSIS, 3DView) and "Example queries" (Saturn in March 2012). A "Help" section is also visible at the bottom right.

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

Show 10 entries

Column visibility Show all Hide all

Select All in current page Reset Selection

granule_uid	dataproduct_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

Questions Discussion on SSHADE

- ??

SSHADE infrastructure development

Databases infrastructure (years 1 – 3)

- Development of SSDM-BL (Band List data model)
- Development of the common 'band list database'
- Import / Search / visualization / Export interface

VO interoperability

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

SSHAE partner's database development

- **Add 10-12 new databases**

The new partners

- ✓ **7 new selected groups**

- **University of Helsinki Astrophysical Scattering and Spectroscopy Laboratory**, University of Helsinki (UH-ApS), FI 
- **Planetary Sciences and Astrobiology**, National Technical University of Athens (NTUA), GR 
- **Laboratório de Astroquímica e Astrobiologia**, UNIVAP university (LASA), São Paulo, BR 
- **Astrophysics Laboratory** University of Salento (UniSalento), Lecce, IT 
- **Planetary Science Institute**, School of Earth Sciences, China University of Geosciences (LPRS), Wuhan, CN 
- **Space Geodesy Group**, Finnish Geospatial Research Institute (FGI), Masala, FI 
- **Centre de Recherches Péetrographiques et Géochemiques**, University of Lorraine, Nancy, FR 

- ✓ **Call for 3 - 5 additional partners (2022)**

Presentations of the New Partners

- **University of Helsinki Astrophysical Scattering and Spectroscopy Laboratory**
- **Planetary Sciences and Astrobiology**
- **Laboratório de Astroquímica e Astrobiologia**
- **Astrophysics Laboratory**
- **Planetary Science Institute**
- **Space Geodesy Group**
- **Centre de Recherches Pétrographiques et Géochimiques**

SSHADE infrastructure development

Databases infrastructure (years 1 – 3)

- Development of SSDM-BL (Band List data model)
- Development of the common 'band list database'
- Import / Search / visualization / Export interface

VO interoperability

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

Bandlist of molecular solids: definition

- **Bandlist:**

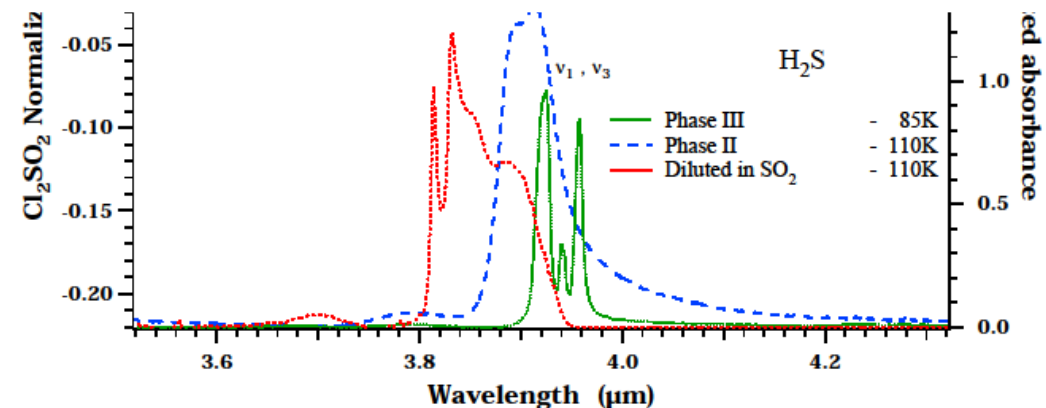
List of band parameters and vibration modes of a **molecule**

- in a simple molecular **constituent** (2-3 species maxi)
- with a defined **phase** and **composition**
- ✓ includes bands of all isotopes
- ✓ for different environments (T, P, ...)

Exemples

H₂S in:

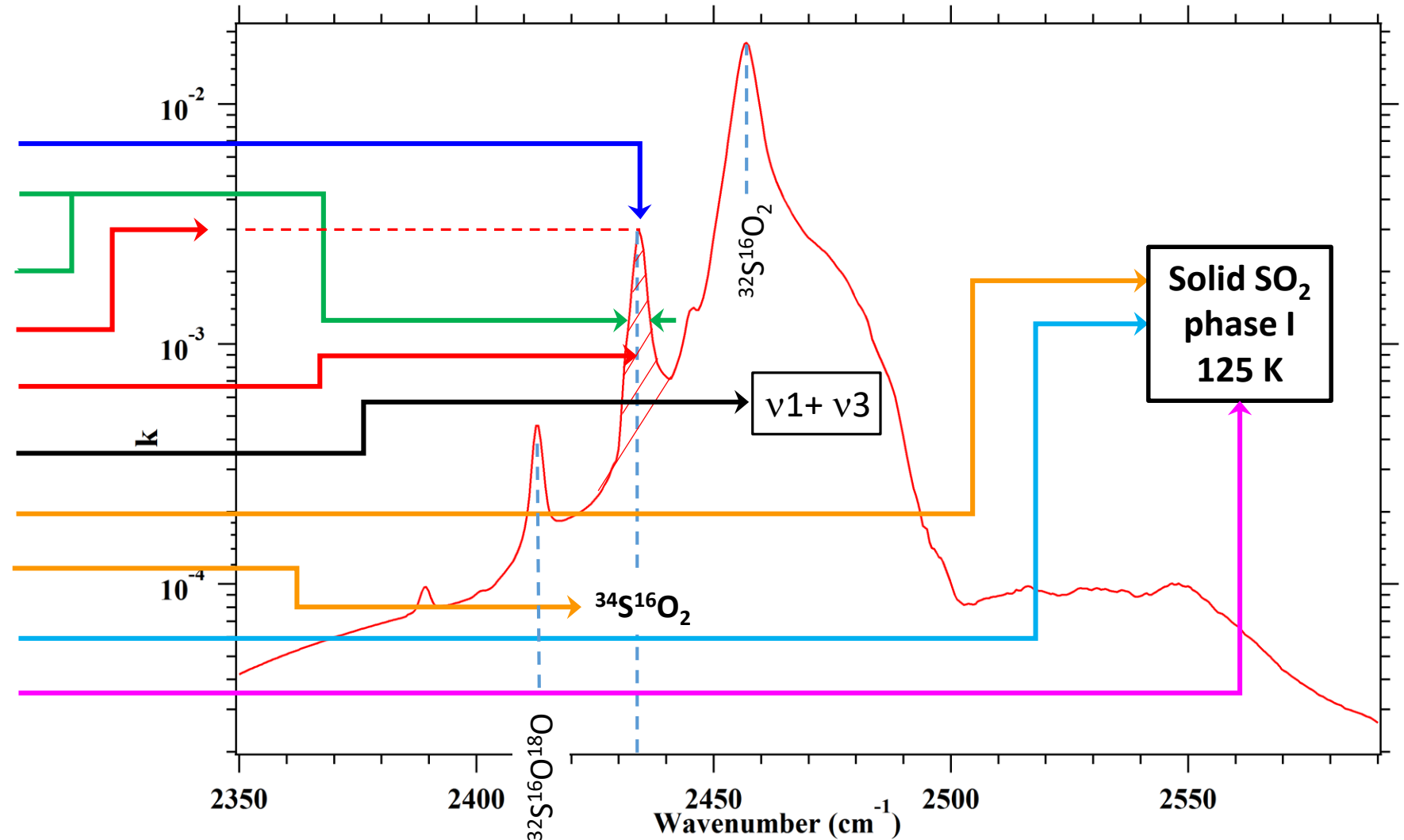
- solid H₂S – phase II
- solid H₂S – phase III
- in crystalline solid SO₂
- in amorphous H₂O
- H₂S clathrate hydrate



Bandlist of molecular solids: band parameters

Bands parameters

- parameters
- Position (energy)
 - Width
 - Shape
 - Peak intensity
 - Integrated intensity
- Quality Constituent
- Vibration mode
 - Molecule
 - Isotope
 - Phase
 - Environment cond.
- Quality / evaluation
- Accuracies
 - Quality / evaluation



Band list of molecular solids in SSHADE

Europlanet-2024 RI (2020-2023)

➤ Development a bandlist datamodel and database

(~ Done)

➤ Development of:

(In progress)

- Search tool
- Visualization tool
- Export tool
- Links to/from spectra

➤ Filling of the database

(To be done)

Review the available data for molecular solids

(Starting)

Prototype delivered (online)

➔ end summer 2021

Final version

➔ end 2022

Euromplanet 2024-RI link with TA2 Activities

TA – Trans National Access

TA2: The Distributed Planetary Simulation Facility (DPSF)

‘Cold Surfaces Spectroscopy Facility’ (<http://cold-spectro.sshade.eu>)

- Perform spectroscopic experiments with our systems
 - **Spectro-gonio radiometre + cryo cells**
 - **Micro-goniometre ‘Gognito’ for dark samples**

Data

- Need to provide their data in open-access after 1-2 years
 - ➔ Stored in the special CSS database @ SSHADE (or in partner DB)
 - ➔ Set ‘public’ after 1-2 years

Euromplanet 2024-RI link with TA2 Activities

TA – Trans National Access

TA2: The Distributed Planetary Simulation Facility (DPSF)

‘Cold Surfaces Spectroscopy Facility’ (<http://cold-spectro.sshade.eu>)

- Perform spectroscopic experiments with our systems
 - Spectro-gonio radiometre + cryo cells
 - Micro-goniometre ‘Gognito’ for dark samples

Call #2 just issued !

Deadline : 6th January 2021

1-2 weeks, Simple proposal, high chance of success, fully paid !

SSHAE partner's database development

- **Add 10-12 new databases**

The new partners

- ✓ **7 new selected groups**

- **University of Helsinki Astrophysical Scattering and Spectroscopy Laboratory**, University of Helsinki (UH-ApS), FI 
- **Planetary Sciences and Astrobiology**, National Technical University of Athens (NTUA), GR 
- **Laboratório de Astroquímica e Astrobiologia**, UNIVAP university (LASA), São Paulo, BR 
- **Astrophysics Laboratory** University of Salento (UniSalento), Lecce, IT 
- **Planetary Science Institute**, School of Earth Sciences, China University of Geosciences (LPRS), Wuhan, CN 
- **Space Geodesy Group**, Finnish Geospatial Research Institute (FGI), Masala, FI 
- **Centre de Recherches Péetrographiques et Géochimiques**, University of Lorraine, Nancy, FR 

- ✓ **Call for 3 - 5 additional partners (2022)**

What does it mean to have a database in SSHADE ?

- **You get:**

- A database (unlimited storage) => **it is YOUR database**
- A large set of tools to prepare, import and manage your data
- Support from the SSHADE team for :
 - Initial training
 - Help for setting up specialized templates, for solving data import difficulties, ...
 - Interface bug correction
 - Improvement of data model or interface to best search / display your data

- **For your database:**

- Full rights to import new data or new version, correct your data ...
- Add and manage the rights of your providers
- A database reference and a DOI
- A specific search page in SSHADE (you can use it from your own web page)
- An information page about your database in SSHADE Wiki

What does it mean to have a database in SSHADE ?

- **For each of your experiments** (set of spectral data):
 - a data reference
 - a DOI
 - A link with your publication
- **For all your data:**
 - A permanent and well documented storage
 - powerful user interface to search / visualize / export interface
 - The SSHADE user community
 - the advertisement made by SSHADE

How do SSHADE compares with other repositories

- General repository (like Zenodo)
 - ❖ Little keywords (and very generic) to describe your data and metadata
(mostly insufficient without associated paper)
 - ❖ Poorly efficient research tool
 - ❖ Mostly findable through the DOI link of the paper
 - ❖ No tool to visualize the data
 - ✓ But free to store, free to recover and you get a DOI
- Editor repositories
 - ❖ No keywords to describe your data
 - ❖ You are not sure your data will be free
 - ❖ Extremely poor search tool (they sell search !)
 - ❖ No tool to visualize the data
 - ❖ Mostly findable through the DOI link of the paper

The advantages of SSHADE

- ✓ An unique data model specialized in our fields (Solid + Spectroscopy)
 - Lot of structured keywords
- ✓ Very efficient search tool specialized in our fields
 - Lot of search filters
- ✓ Provide to the user all information on sample, spectra, instruments, publications, ...
- ✓ Provide to the user even more information (detailed info on molecules, minerals, ...)
- ✓ Tools to visualize and do some measurements on the spectra (+ more later)
- ✓ Data can be downloaded in a variety of customized units & formats

- ✓ SSHADE is an official member of DataCite (DOI attribution)
- ✓ You get (for free) a data reference and a permanent DOI
- ✓ Your data are referenced by browsers (with relevant keywords) => increase data citation ?
- ✓ SSHADE follow the 'FAIR' principles (**F**indability, **A**ccessibility, **I**nteroperability, **R**euse)
- ✓ Should be in some near future 'a certified database'
- ✓ There is an increasing 'SSHADE users' community : over 220 people registered

But this has some cost !

- Lot of scientific and technical developments
 - Datamodel
 - Import / search /visualization / export tools
 - DOI, VO, ...
- Detailed metadata to provide (but only the one you know !)
 - some import files are big, but will be simplified for your specific case
- A data import training is necessary
- **But you will get support** from the SSHADE team
 - Help for setting up specialized templates
 - For advices on how to organize your data
 - for solving data import difficulties, ...
 - Interface bug correction
 - Improvement of data model or interface to best search / display your data

Discussion/questions on partner's database

- ??

Task of the of the SSHADE 'Support'

SSHADE Database support

- Train the managers to prepare and import their spectroscopic data in SSHADE
- Support the managers and contributors to prepare and import their data
- Help (in-situ and on-line) on preparation and validation of data ingestion files.
- Prepare customized data templates for their specific samples and experiments.

- Develop tutorials and documentation for SSHADE managers and providers
- On-line support to each database manager

- Help feed data collected by the visitors of TNA on spectroscopic instruments

Task of the of the SSHADE 'Support'

SSHADE fundamental database feeding

- Preparation and feeding of the fundamental data of SSHADE
(molecules, minerals, meteorites, ...).
 → preparation on request by the partners
- Management of these data.

Band List database feeding

- Contribute to the preparation and feeding of the common 'band list' database.
- Compilation and critical review of the absorption band parameters of a series of simple molecular ices and minerals from data of the SSHADE partners + bibliography.

Task of the of the SSHADE 'Support'

Coordination of consortium

- Animation of SSHADE consortium
- Advertisement of SSHADE and its data

Support to users

- Preparation of documentations for users
- Develop tutorials for SSHADE users
- Training for users at conferences
- On-line support

Tasks of the Scientific Managers and Database Managers

- **Scientific manager**
 - define which data will be provided to the database
 - scientific validation of data
 - animation of his data base
 - contribution to the common « Band list » database
- **Data base manager**
 - prepare and test import files (all types)
 - import data (sample, spectra, matters) + corrections
 - report bugs, data errors and improvements
 - Trains additional data providers
- **Data producers**
 - Prepare the metadata information and the data file
 - help prepare and test import files for their data
 - Can import / correct data (if allowed)
 - Validate imported data

Discussion/questions on tasks

- ??

Training session of managers for SSHADE partners

Aims

To be able to fill the import xml files and import / correct the data

Program:

- Understanding the SSHADE infrastructure
- Understanding the SSDM data model
- Preparing XML import files
- Validation and import data
- Correct data
- Customization of the import files to your type(s) of data

Mostly practical's

- Duration : 2.5 days

Training session of managers

- Preparation of basic information and metadata
 - Database
 - Laboratory
 - Experimentalists
 - Instruments
 - Publications
- Preparation of spectral data and metadata
 - Local matters
 - Samples
 - Experiments
 - Spectra

Feedback from “Mirabelle” Team



- Trained ‘on-line’ 3-5 November 2020
- Used mineral soil measured in field in Atacama (georeferencing)

Database implementation by partners

- Preparation of fundamental data by SSHADE
 - Provide list of fundamental data to be used:
 - Molecules, (atoms)
 - Minerals, simple solids
 - Meteorites
 - Standard matters
 - Contribute to document them
- Define Who do what in your lab (which part of the work, ...)
- Define your feeding plans (which data, ...)
- Found an ACRONYM and a Name for your database (+ Logo)

Planning training Database managers

2021

(to be defined)

- January
- March
- May
- July
- October
- December

Questions on database implementation and training

- ?

- ➔ Send your preferences of month(s) (will make a 'doodle')

- ➔ Send me your presentation

- ➔ I can send to who want the preparatory material with the first files to fill