# The long history of the development of the Solid Spectroscopy Data Model of SSHADE

Bernard Schmitt

IPAG – CNRS/UGA

# A little bit of history: from past to future

- 2002-2006: Idea ... Concept ... Content demonstrator: **STSP**
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Addition of 7 databases from around the world

# STSP : Spectroscopie et Thermodynamique des Solides en Planétologie et astrophysique

- 2002 – 2006

STSP pour le Centre de Données sur les Surfaces Planétaires (CDSP) …

dans le cadre de la préparation des missions spatiales d'observation des surfaces par imagerie, spectroscopie ou spectro-imagerie

- ✓ DISR-VIMS/Huygens-Cassini, OMEGA/Mars Express, VIRTIS/Rosetta, …

➔ bases de données Web sur les propriétés **physiques** et **spectroscopiques** des solides moléculaires planétaires et astrophysiques.

➔ Données du LPG + bibliographie

# STSP: Premiere idée de base de données de “solid spectroscopy and thermodynamics”

Très simple et limité:

- Mesures en transmission (+ absorption coefficient, constantes optiques)
- Mesures en réflectance
- Propriétés thermodynamiques

- était vu initialement comme:
  - un stockage local de nos données de labo et de nos publications
  - La mise en public des données publiées

- **2003: Les propriétés qui y seront inclues sont:**

  + **Généralités:**
    - nom, formule, masse molaire, isotopes
  + **Cristallographie**
    - phases, structure cristalline
    - densité
  + **Thermodynamique**
    - diagramme de phase (pur, mélange, solide-liquide, hydrates, clathrates, ...)
    - pression de vapeur
    - chaleur latente, capacité calorifique
    - conductivité thermique
  + **Spectroscopie**
    - électronique
    - vibrationnelle (spectres, fréquence, intensité, modes, Cte anharmonique, ...)
    - Raman
    - constantes optiques
    - indice de réfraction
  + **Références bibliographiques sur les solides**
  + **Observations astrophysiques**
    - Objet, état, bande, température, ...
    - références bibliographiques

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# STSP: Premier développement de base de données de “solid spectroscopy and thermodynamics”

- Phase de maturation des idées et concepts et de tri des priorités !

  … faute de moyen de développement !

  - nombreuses discussions, conseils, … choix !

  - nombreuses questions fondamentales, ex :

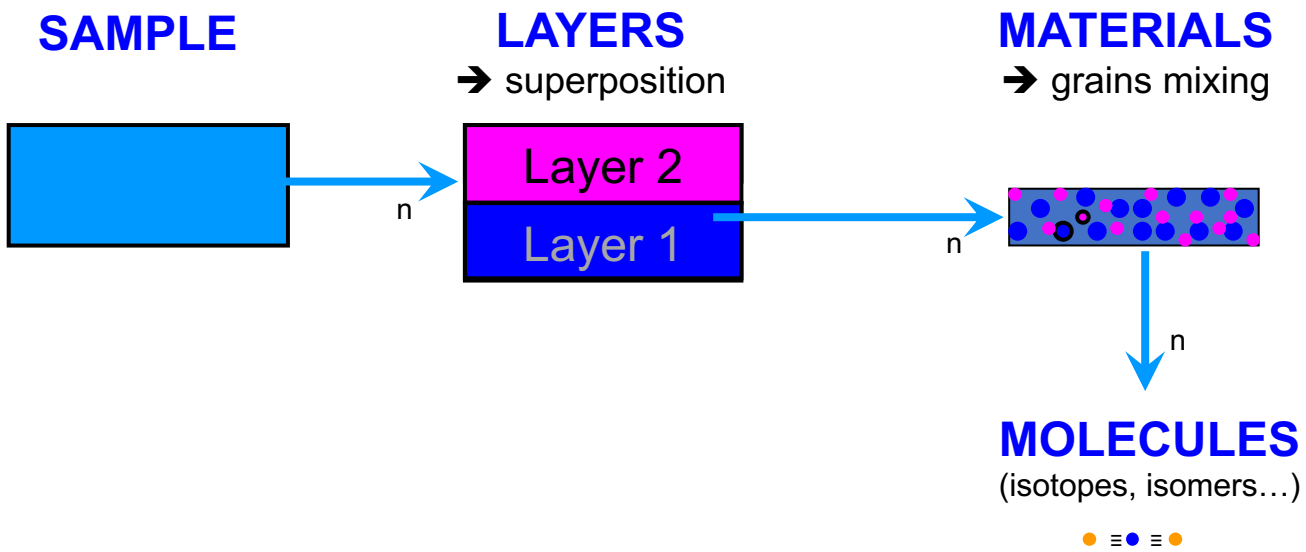
    - ✓ Faut-il créer ‘ex nihilo’ un modèle de donnée ?
    - ✓ C’est quoi un échantillon ?
    - ✓ Comment les décrire de façon commune et objective ?
    - ✓ aussi données d’autres groupes ?

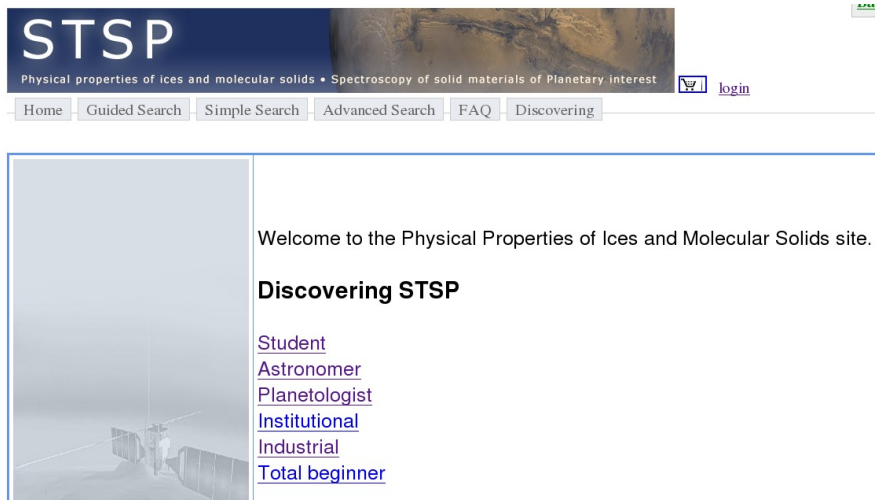
➔ Démonstrateur de modèle de donnée et de contenu sous SPIP !

# STSP: Premier développement de base de données de “solid spectroscopy and thermodynamics”

- Premier développement de data model et d’interface

- Première structuration du ‘sample’



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  Addition of 7 databases from around the world

# GhoSST : 1ère phase de développement (Programme Europlanet RI)


- 2009 : Europlanet + OSUG = des moyens financiers et humains !

Base de données du LPG

« Grenoble astrophysic and planetology Solid Spectroscopy and Thermodynamics »

Modèle de données :

➔ Champ restreint aux spectroscopies du LPG

mais déjà **large en gamme** (Vis-IR lointain) et **techniques** (transmission IR, Reflexion Vis-NIR, µ-Raman, Fluo, spectro-imagerie microscopique MIR, …)

et sur une **grande variété de solides** (glaces, minéraux, organiques, météorites, …)

➔ mais avec en tête l'idée d'une extension à d'autres données d'autres groupes

# GhoSST : 1ère phase de développement (Programme Europlanet) RI

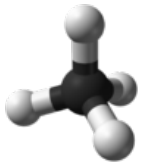
- Maturation et structuration du modèle de données

➔ SSDM (Solid Spectroscopy Data Model)

✓ Une meilleure structuration des tables
✓ Une description plus complète et généraliste des échantillons …
(ajout des ‘constituents’ et des ‘matters’)
✓ Une extension des options d’expériences et de spectres …
✓ Ajout d’une ‘bandlist’ et ses ‘molecular parameters’ très simple

➔ Création des interfaces d’import/recherche/visualisation/ export

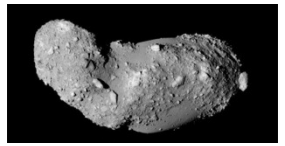
# SSDM General Structure

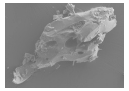


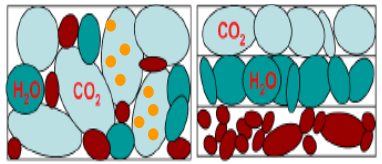
SPECIES

MATTERS

OBJECTS

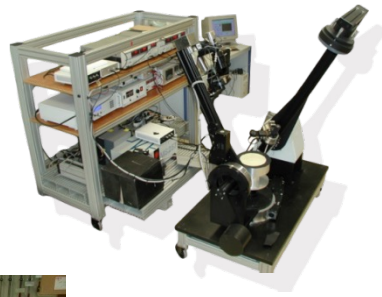


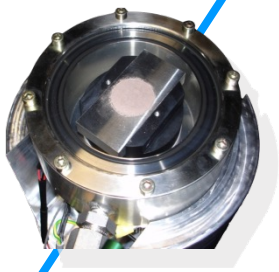




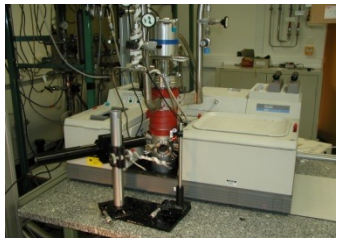

SAMPLE

INSTRUMENT



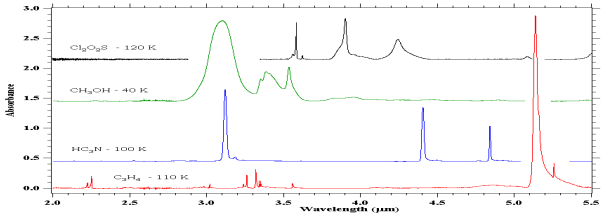


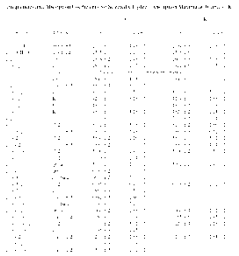
EXPERIMENT



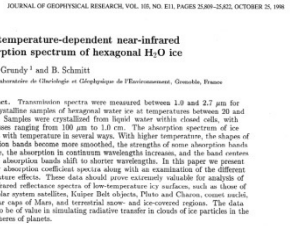
BAND LIST

SPECTRA



PUBLICATIONS



The temperature-dependent near-infrared absorption spectrum of hexagonal $H_2O$ ice

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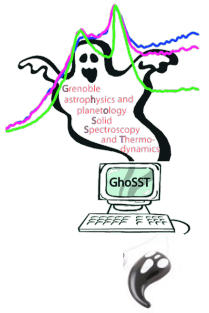
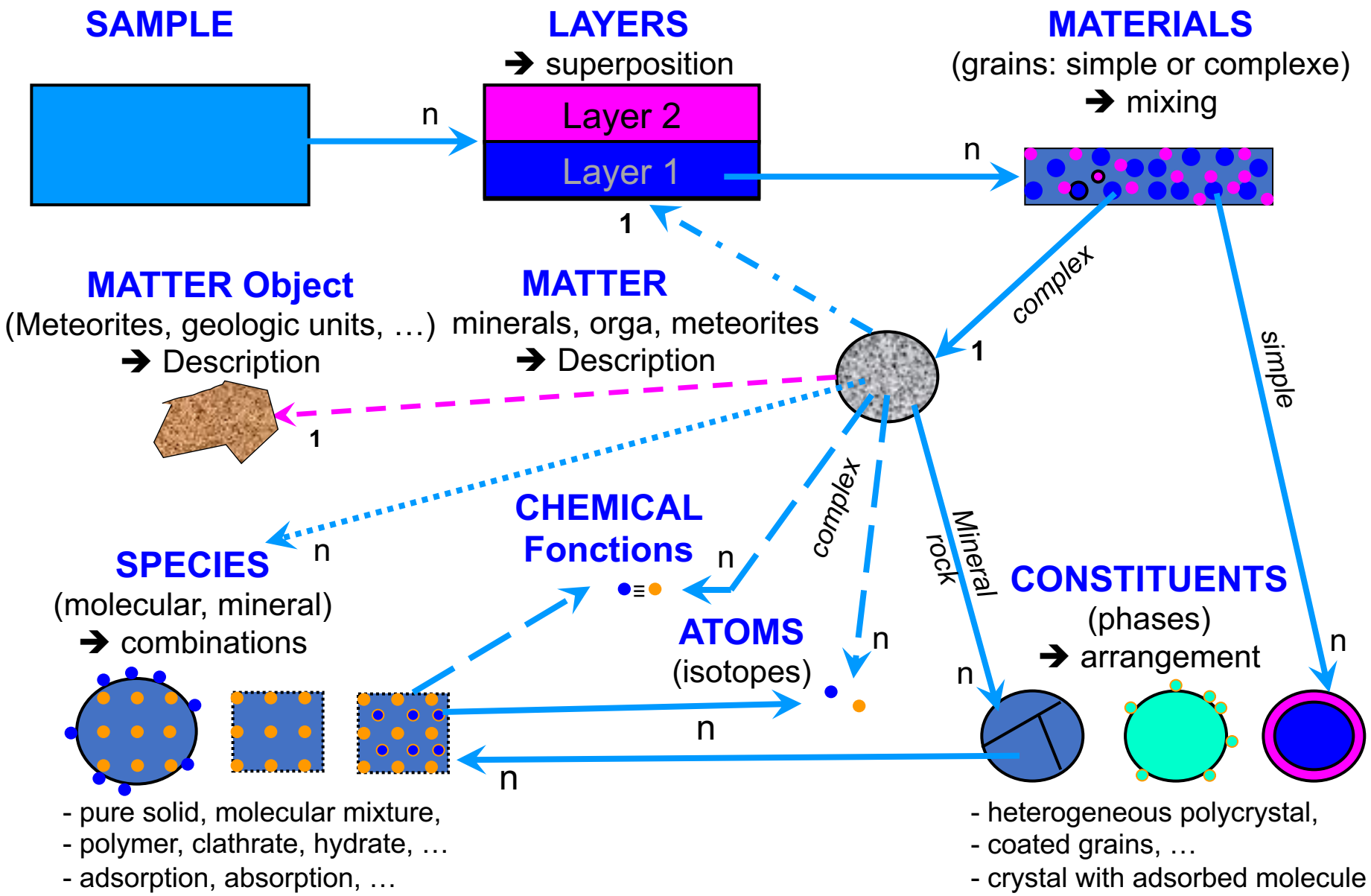


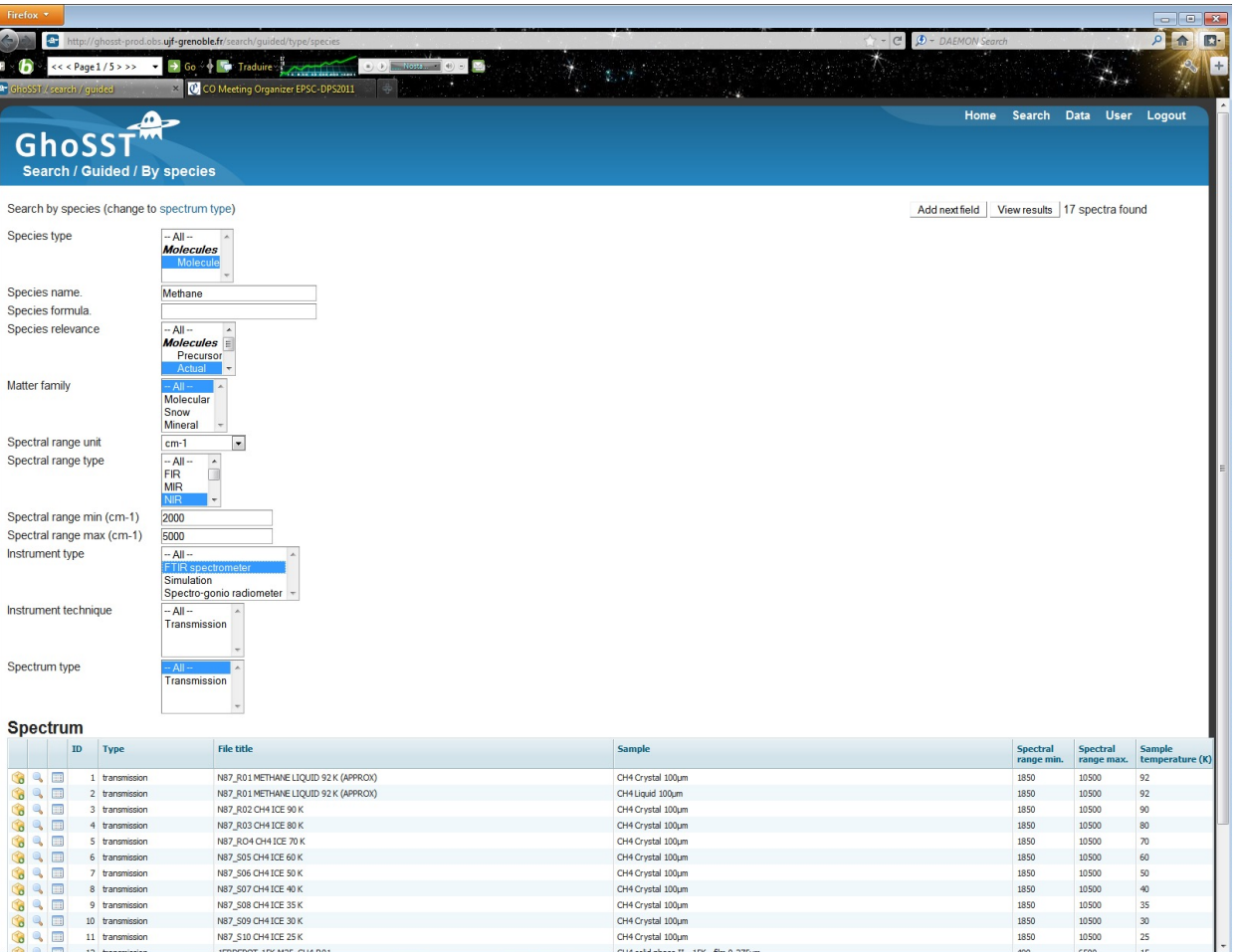
# SSDM: Solid Sample description

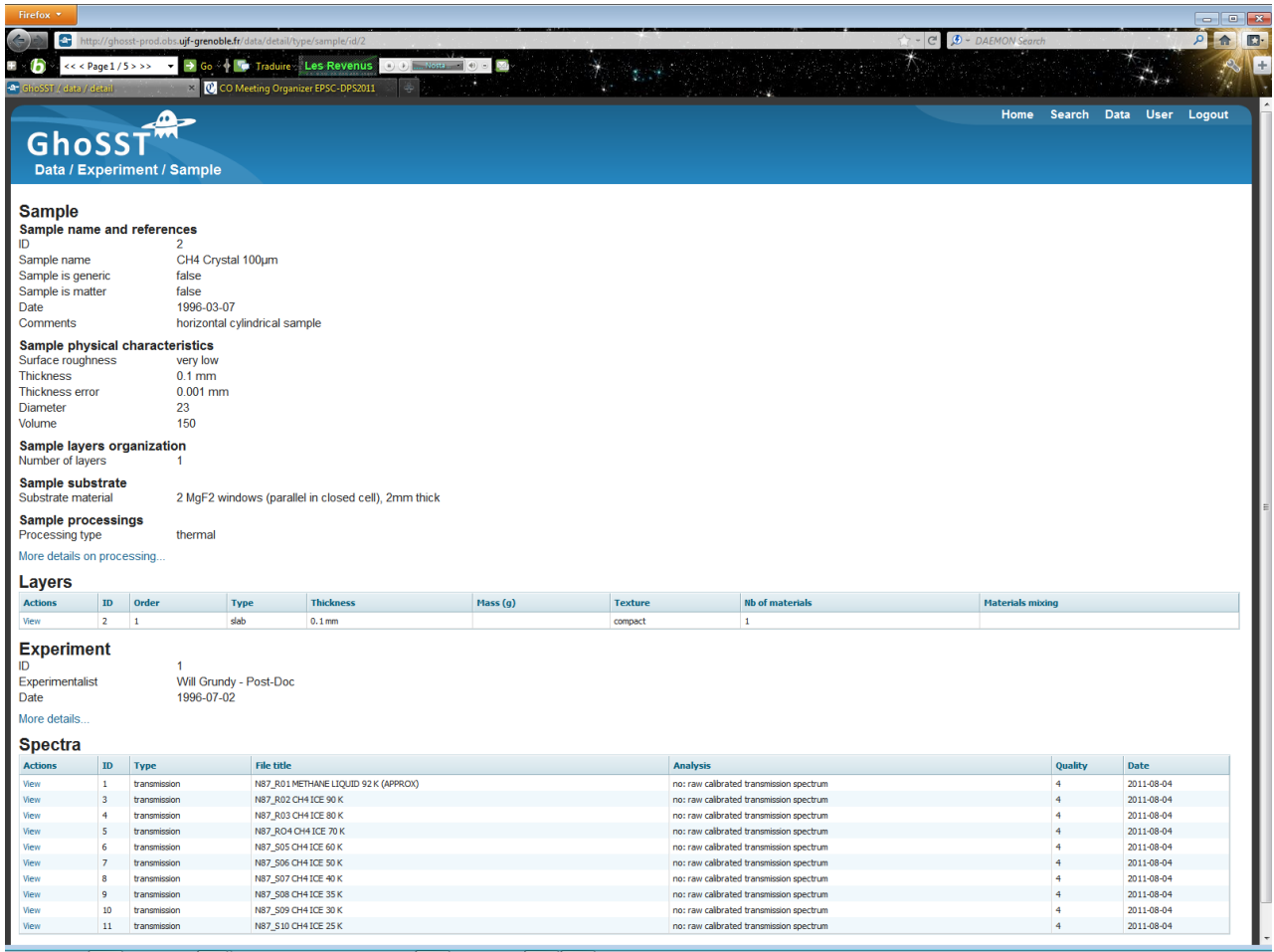
*The most complex part for solids !!!*



# GhoSST : La 1ère phase de développement (Programme Europlanet RI)

➔ Mise en ligne le 25 Septembre 2012



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- Extension des buts de SSHADE
  - ➔ Adaptation à une infrastructure de bases de données
- Extension des types de données
  - ➔ Extension du modèle de données SSDM

# 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**

➔ **set of spectral databases** from a Consortium of research groups

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

✓ **Develop** tools & interface to provide on-line the experimental data

✓ **Develop** tools to analyze and use the data

GhoSST

Fame

LayeredSilicatesDatabase

BYPASS

Bern icY Planetary Analogues

# Main aims 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…**

# SSHADE : 2ème phase de développement (Programme Europlanet-2020 RI)

- Extension des buts de SSHADE

  ➔ Adaptation à une infrastructure de bases de données

- Extension des types de données

  ➔ Extension du modèle de données SSDM

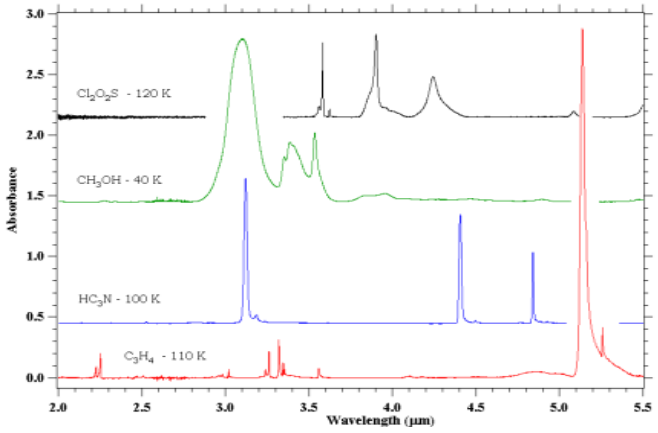
  ✓extension des options
  - d'échantillons (phases fondamentales, bonds, matter organic…)
  - d'expériences
  - de spectres (BRDF, XANES, …)

  ➔ Énorme travail de remaniement des fichiers existants !! (6 mois de travail… !)

  ✓ Mise de coté provisoire des bandlists

# 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**



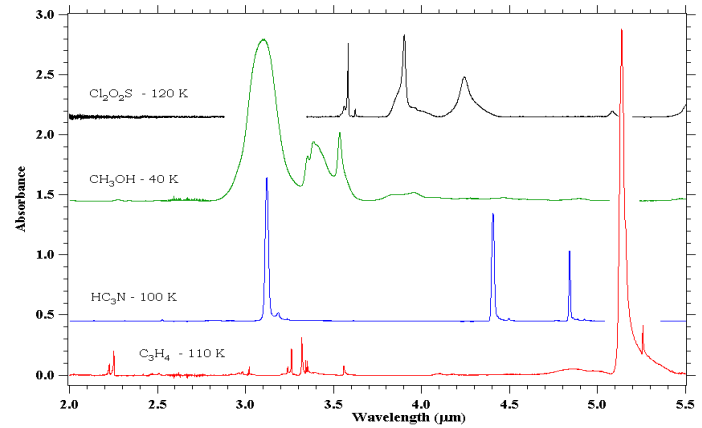

- **Samples**
  - **Synthesized** in the laboratory
  - **Natural terrestrial analogues** collected or measured in the field
  - **Cosmomaterials collected on Earth**: (micro-)meteorites, *IDPs,* …
  - **Extra-terrestrial samples** collected on planetary bodies: lunar soils…

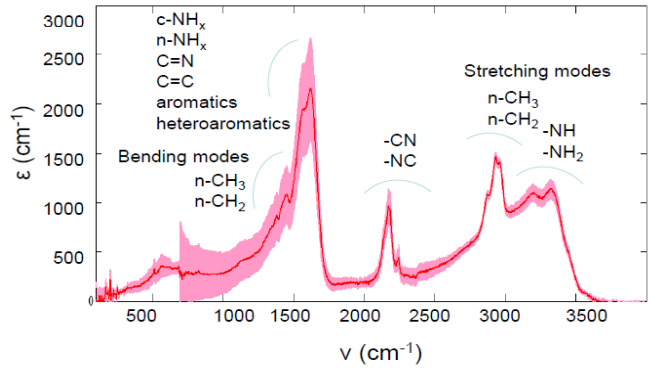
# Which types of spectra in *SSHADE* ?

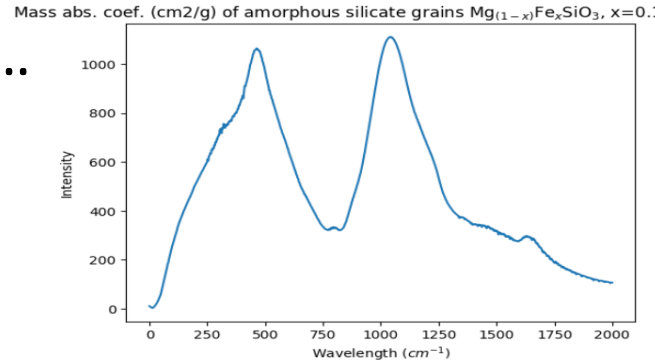
- **Spectral ranges:**
  - Designed from γ-rays to radio wavelengths
  - Now mostly **from VUV to sub-mm (0.2µm - 1mm),** plus **X-rays**.

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

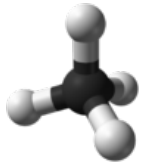
➢ **Spectra**
  - **Transmission** spectra, absorption coefficients,
  - **Optical constants** …
  - **Reflectance** spectra of surfaces, spectro-photometric functions, …
  - **Raman** spectra & micro-spectroscopy, *Fluorescence*, …
  - **XANES** spectra



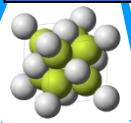



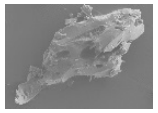



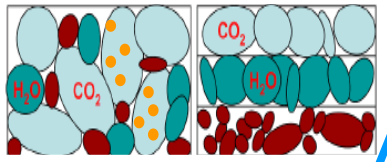
# SSDM General Structure



SPECIES → PHASES → MATTERS ← OBJECTS ← BODIES

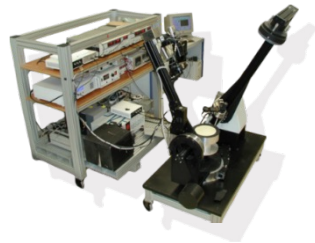


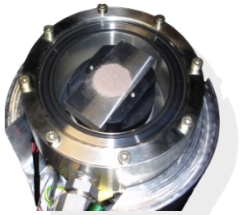





SAMPLE

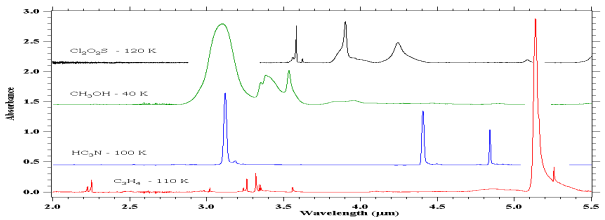
INSTRUMENT

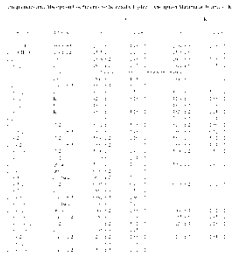


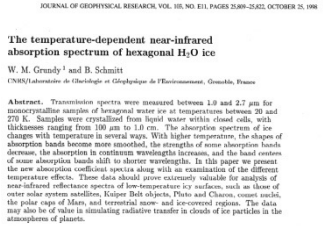


EXPERIMENT ← EXPERIMENTALIST

BAND LIST ← SPECTRA → PUBLICATIONS





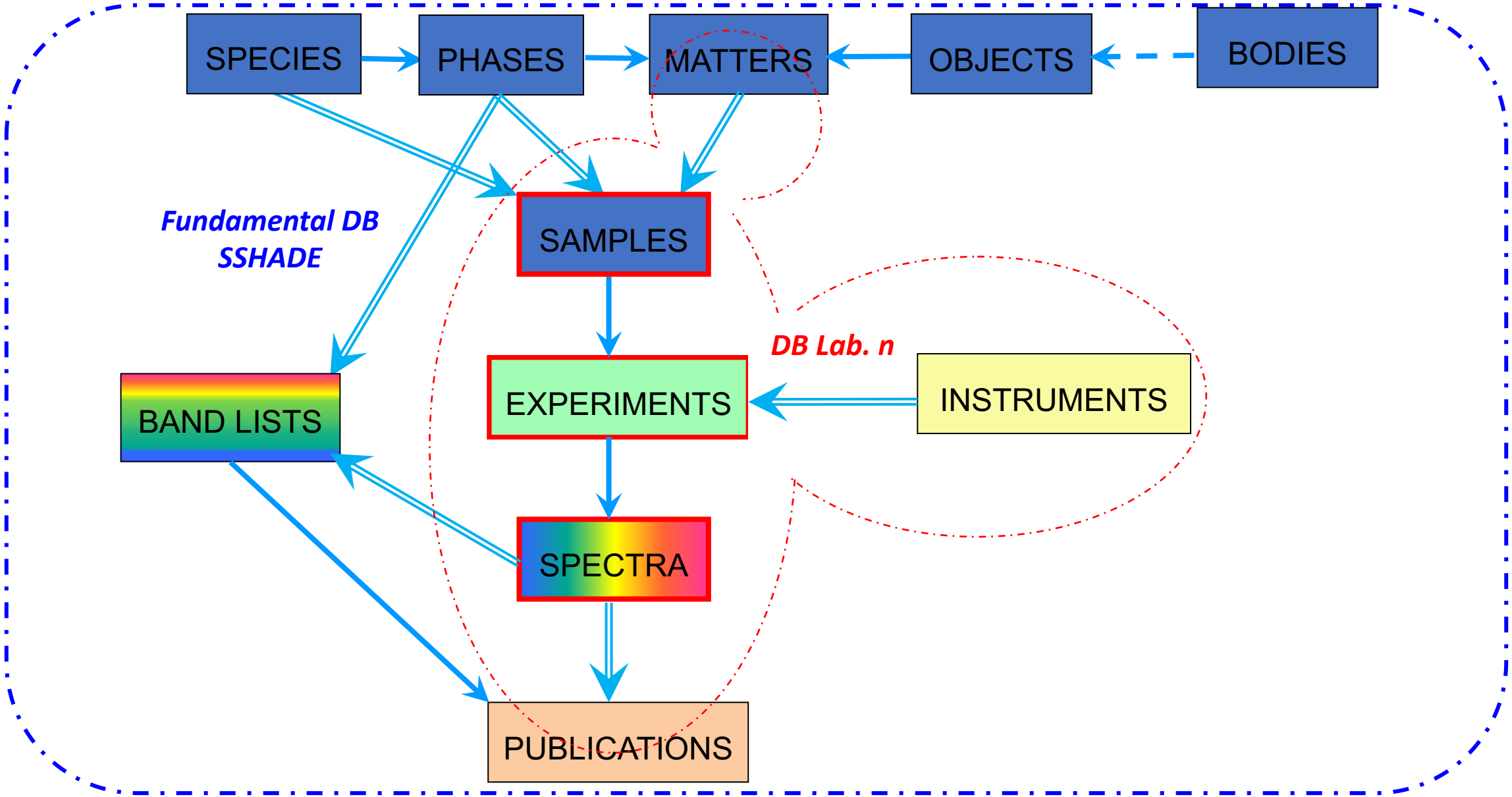
JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 103, NO. E11, PAGES 25,809–25,822, OCTOBER 25, 1998

**The temperature-dependent near-infrared absorption spectrum of hexagonal $H_2O$ ice**

W. M. Grundy [1] 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 monocrystalline 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 shapes of absorption bands become more smoothed, the strengths of some absorption bands decrease, 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.

# SSHADE: new SSDM structure



# SSHADE-Spectra : 2ème phase de développement (Programme Europlanet-2020 RI)

- Extension des buts de SSHADE

  ➔ Adaptation à une infrastructure de bases de données

- Extension des types de données

  ➔ Extension du modèle de données SSDM

  ✓extension des options
  - d'échantillons (phases fondamentales, bonds, matter organic…)
  - d'expériences
  - de spectres (BRDF, XANES, …)

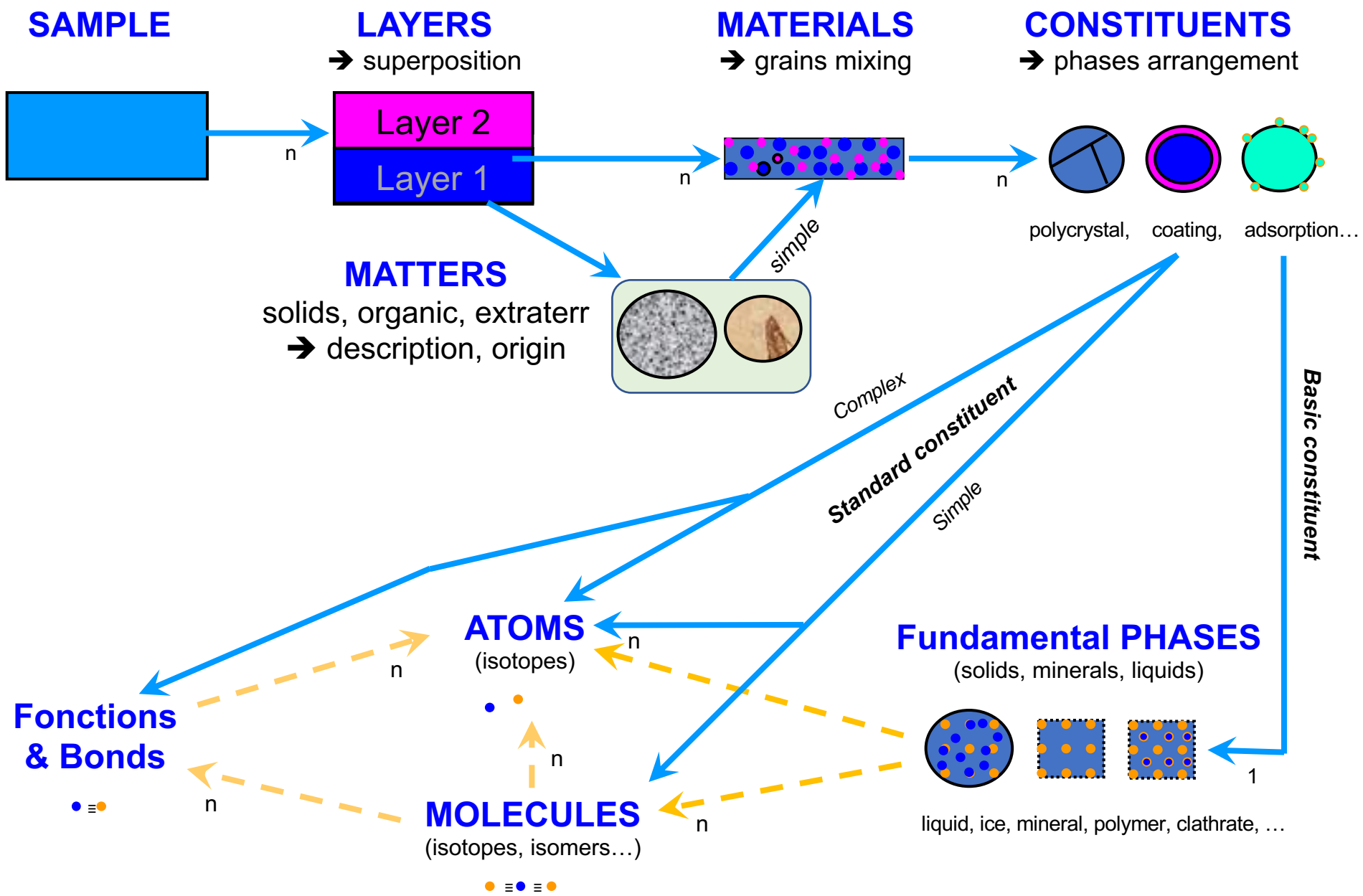
  ➔ Énorme travail de remaniement des fichiers existants !! (6 mois de travail… !)

  ✓ Mise de coté provisoire des bandlists

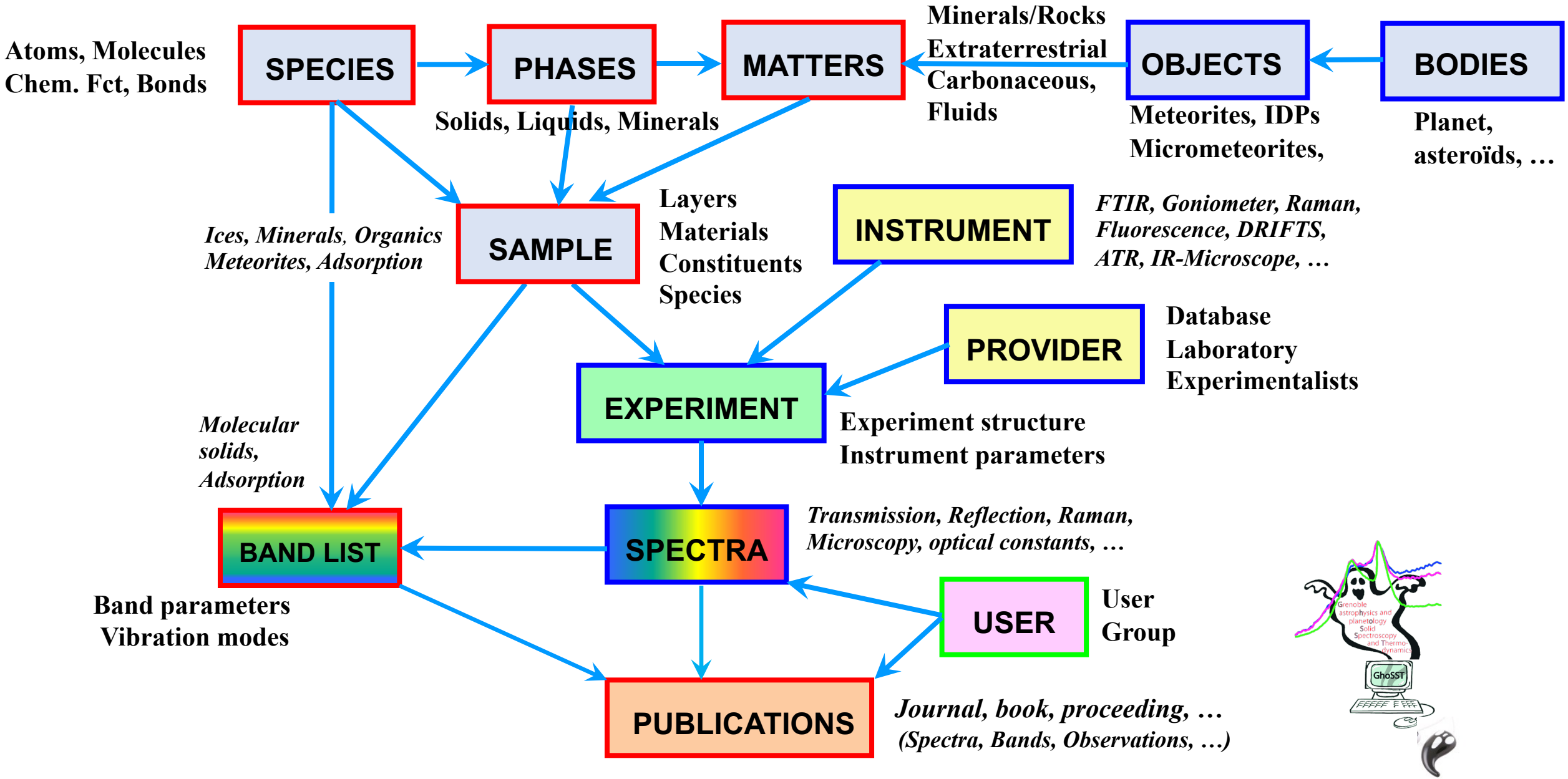
  ✓ restructuration poussée des tables
  ✓ homogénéisation des descriptions et options

  ➔ Mise en ligne de SSHADE-Spectra avec 10 bases de données: 1er Février 2018

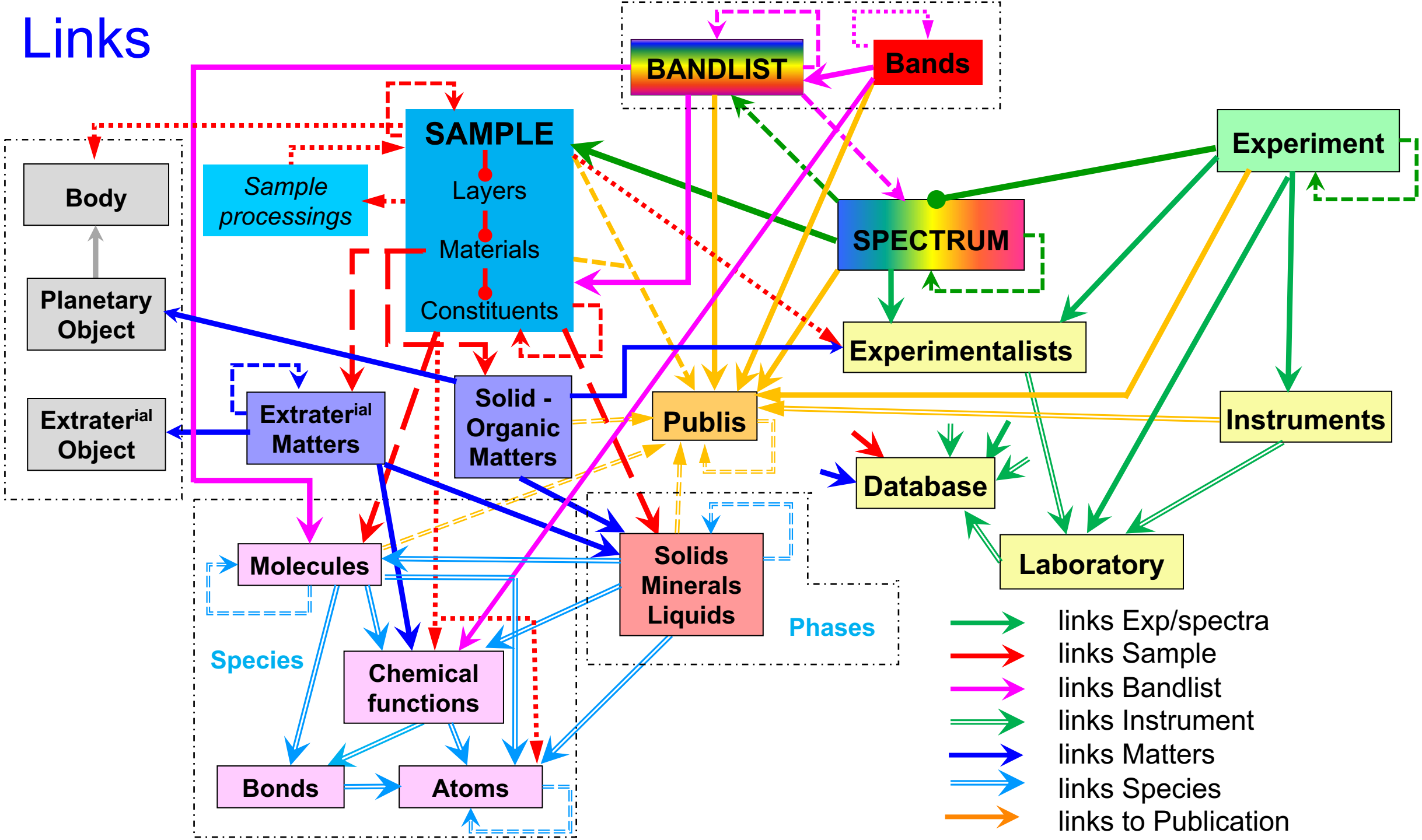
# SAMPLE description: Layer(s) / Material(s) / Constituent(s)



# SSDM General Structure



# Links


BANDLIST
Bands
SAMPLE
Layers
Materials
Constituents
Sample processings
Experiment
SPECTRUM
Body
Planetary Object
Extraterial Object
Experimentalists
Extraterial Matters
Solid - Organic Matters
Publis
Instruments
Database
Laboratory
Molecules
Solids Minerals Liquids
Phases
Species
Chemical functions
Bonds
Atoms
links Exp/spectra
links Sample
links Bandlist
links Instrument
links Matters
links Species
links to Publication

# 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: **Development** (Europlanet + VAMDC – FP7) of:
  **SSDM** (Solid Spectroscopy Data Model) and **GhoSST database**
- 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 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)
- Nov. 2020: SSHADE with 17 active databases (> 3300 spectra)
- ✓ 2020-2024 **Europlanet-2024 RI** : **development of ‘band list of solids’ database** (online: August 2021)
  Addition of 7 databases from around the world

# SSHADE-Bandlist : 3ème phase de développement (Programme Europlanet-2024 RI)

- Ajout d'une base 'commune' de liste de bandes
  ➔ description très différente des spectres

- Une autre philosophie
  ➔ compilation critique des données + sélection

- Une description spécifique s'appuyant sur l'existant

  ➔ Création du modèle de données SSDM-Bandlist

  - ✓ basé sur les constituents
  - ✓ cherchant à être compatible avec VAMDC (gaz)
  - ✓ mais plusieurs différences physiques et de concept

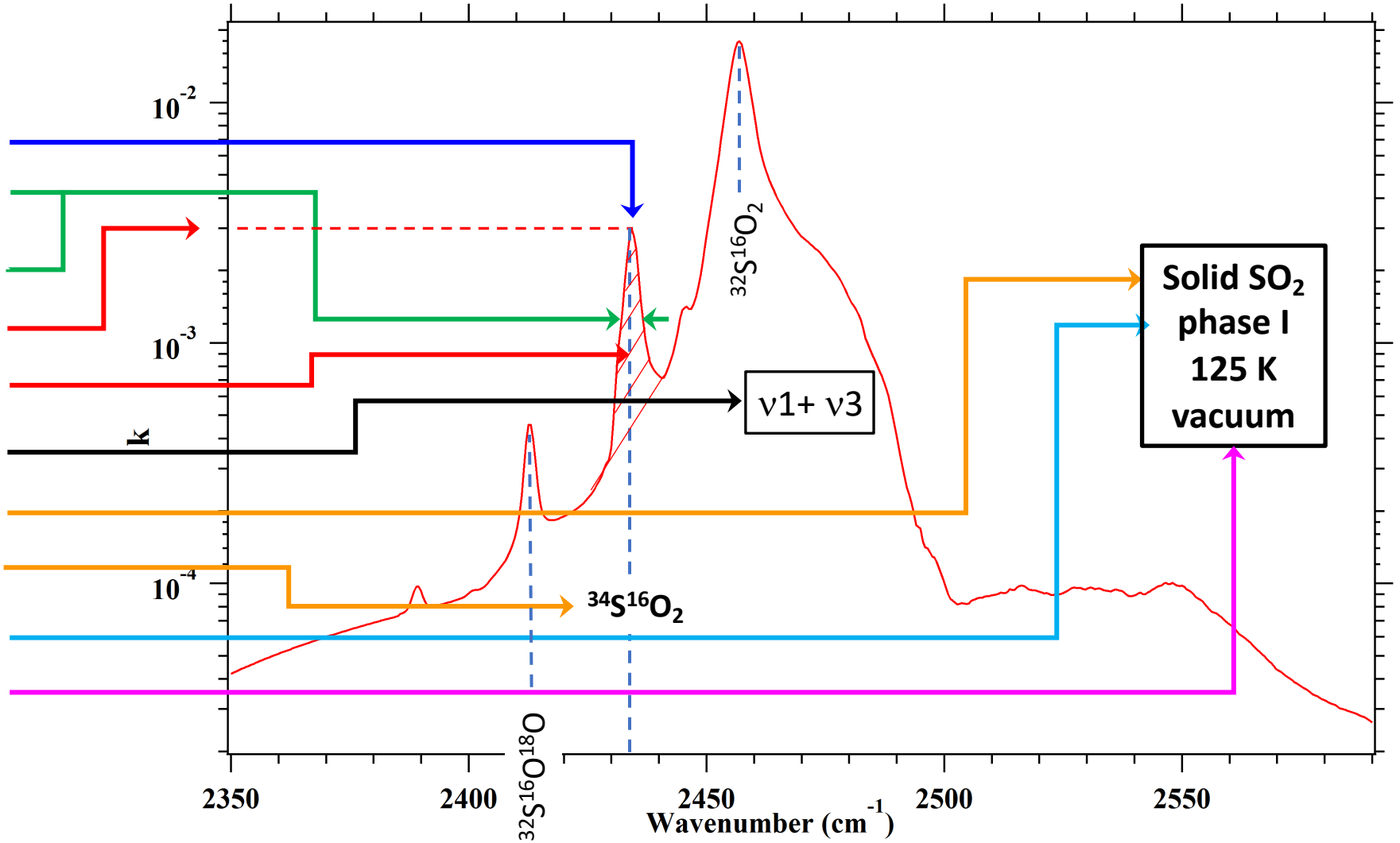
# Band list of solids: band parameters

## Bands parameters

*parameters*
- Position (energy)
- Width
- Shape
- Peak intensity
- Integrated intensity
- Vibration mode

*Constituent*
- Molecule
- Isotope
- Phase
- Environment cond.

*Quality*
- Accuracies
- Quality / evaluation



# SSHADE-Bandlist : La 3ème phase de développement (Programme Europlanet-2024 RI)

- Ajout d'une base 'commune' de liste de bandes

➔ Création des interfaces d'import/recherche/visualisation/ export

➔ Mise en ligne publique Aout 2021

# Some points on DM development

- SSDM is now a powerful, yet complex, datamodel for solid spectroscopy covering a very wide range of type of samples, spectra and experiments

  ✓ Almost no new case of samples or experiment failed to be described, except the types still planned!
  ✓ Complexity due to wide range of solids, spectral ranges and spectro techniques

Require:

  ✓ a lot of cumulative and long term effort, a good interaction between scientists and engineers
  ✓ to be well structured and homogeneous
  ✓ to have a clear idea of its possible additional evolution
  ✓ a lot of evolutions during its developments

    some major modification / restructuration ➔ lot of work to upgrade the already imported
  ✓ **a well documented and up-to-date reference document**, well synchronized with the import files (xml) and the developed interface

➔ Part of SSDM may be used by other more specialized databases

# The SSDM document

- **Provide fully detailed and complete info on:**

## Table

- Root name
- General description

## Keyword

| | |
|---|---|
| • Name | [Key-word] |
| • Type (varchar, blob, float, integer, enum, …) | [Type] |
| • Mandatory level | [Level] |
| • Unit | [Unit] |
| • Definition | [Description] |
| • For Enum: list of attribute and their definitions | [Description] |
| • Conditions, constraints | [Description] |
| • Examples, notes, links | [Description] |

It is the REFERENCE document (~750p)
https://wiki.sshade.eu/sshade/documentation/ssdm

# The SSDM document

**Example:**

## 10.6 Material Table

*Root of the table:* ***material***

*Data type*: in 'Sample'

*Note: not* for precursor materials

Conditions

Definition

Keyword

Data type

Mandatory level

Notes and Exemples

| Key-word | Type | Level | Table | Exp | Unit | Description |
|---|---|---|---|---|---|---|
| ***Material import mode and index*** | | [!!O] | | | | *Condition:* absolute mandatory when "*matter_uid*" = Ø |
| *material*_import_mode | enum(text) | P [!!_m] | Mater | (V) | -- | Mode of import of the "Material" metadata<br>Enum: {first import, inherited, use existing, ignore, draft, no change, correction}<br>*For precursor_material:*<br>Enum: {first import, inherited, ignore, draft, no change, correction}<br>*Implied conditions*: when "*material*_import_mode" = 'use existing', only "*material*_uid", and the KWs of "material arrangement and abundance in the layer" are needed.<br>*Definitions:* see "*sample*_import_mode" |
| *material*_index [**][-xml] | int(10) | B [!!_g] | Mater | F | -- | Automatic random but unique number (ID) given to new material |
| *material*_uid [**] | varchar(255) | S0/S1 [!!_m] | Mater | F | -- | Unique identifier code (UID) given to the material table (to be created)<br>*Important note:* when "*material*_import_mode" = 'use existing', this UID is then the "*material*_uid" of an existing material already in the database<br>*Note:* This code name should start with 'MATERIAL_' for layer or matter materials, and be very accurately formatted in order to be simple and unique<br>*Ex:* It should be of the style 'MATERIAL_AB_yyyymmdd_123' where 'AB' are the initials of the person preparing the import, 'yyyymmdd' is full date of the day, and '123' is an incremental order number for that day from '001 to '999' |
| ***Material type*** | | | | | | |
| *material*_is_precursor [-xml] | boolean | S0 [!!_g] | Mater | F | -- | Flag telling if the material is a 'precursor material'<br>BoolEnum: {yes, no} or {true, false}<br>*Definition:*<br>- *Precursor material ('true')*: material used to prepare the final material of a sample or of a matter through a series of processings.<br>- *Normal material ('false'):* material that is part of a final sample or a |

# The SSDM document

**Example:**

| | | | | | | |
|---|---|---|---|---|---|---|
| *material*_grain_size_min | float | S3 [m] | Mater L1 | F | var. | Smallest size (diameter) of material grains of this size range<br>*Unit:* in "*material_grain_size_unit*"<br>• converted in 'm' unit in the database but provided to user in "*material*_grain_size_unit" |
| *material*_grain_size_max | float | S3 [m] | Mater L1 | F | var. | Largest size (diameter) of material grains of this size range<br>*Unit:* in "*material_grain_size_unit*"<br>• converted in 'm' unit in the database but provided to user in "*material_grain_size_unit*" |
| *material*_grain_size_fraction | float | U [m] | Mater L1 | F | *no* | Mass fraction of material grains comprised between size min and size max (diameter)<br>*Note:* value between 0 and 1. |
| *material*_grain_size_fraction_error | float | U [m] | Mater L1 | F | *no* | Absolute uncertainty on the mass fraction of material grains comprised between size min and size max (diameter) |
| *material*_grain_shape | enum(text) | S1b/S2 [m] | Mater L1 | F | -- | Shape of the individual material grains (granular material) or crystals (compact : material) of this size range<br>Enum: {amorphous, irregular, equant, reniform, globular, spherical, flakes, platy, tabular, lathlike, columnar, acicular, capillary, cubic, cylindrical, hexagonal, octahedral, prismatic, pyramidal, rhombohedral, nuggets, botryoidal, dendritic, spheres aggregate, aggregate, fluid, other, unknown}<br>*Definitions:*<br>Simple shapes :<br>- '*amorphous*': no crystalline form or imitative shape<br>- '*irregular*': occurs as irregular, anhedral crystals<br>- '*equant*': shape tends to be convex equidimensional (e.g. feldspars).<br>- '*reniform*': "Kidney like" in shape (e.g.. hematite).<br>- '*globular*': spherical, or nearly so, rounded forms (e.g. wavellite).<br>- '*spherical*': spherical, rounded aggregates.<br>- '*flakes*': flat, thin crystals or aggregates.<br>- '*platy*': sheet forms (e.g. micas).<br>- '*tabular*' : book shape (plagioclase)<br>- '*lathlike*': flat elongate grains (plagioclase)<br>- '*columnar*' : forms columns<br>- '*acicular*': needle-like crystals.<br>- '*capillary*': very slender and long, like a thread or hair (e.g. millerite).<br>Crystalline shapes:<br>- '*cubic*': cubic shaped crystals.<br>- '*cylindrical*': shaped like a cylinder.<br>- '*hexagonal*': six-sided crystal shape in cross-section or habit. |

Unit

Enum attributes list

Enum attributes definitions

# SSDM-Spectra and SSDM-Bandlist interoperability

- **with data cite (DOI)**
  - SSDM made compatible with DataCite datamodel to allow automatic extraction of metadata useful for DOI and associated metadata through simple mapping and conversion
    ➔ necessary to add some administration KeyWords in SSDM

- **with EPN-TAP**
  - More complicated mapping as mostly 2 different fields
    - no sample description
    - VESPA added some keywords for increased interop

    ➔ Spectra: succeeded to get interoperability allowing to discover the spectra
    ➔ Bandlist: Development in progress => new keywords ?

- **with VAMDC**
  - Compatible for part of SSDM-Bandlist
    - mostly description of molecules and some spectroscopic parameters
  - But incomplete for solid constituents
    ➔ need extension of XSAMS before interop
  - also different ways to describe some spectroscopic parameters and some concept differences
    - Ex: solid phonon modes, almost only transition from ground state

# Evolution for RéGEF and for the ‘extended free data’

- RéGEF : will include all experimental laboratories in Earth and planetary Sciences, possibly also astrophysics.
- A **new network on « Spectroscopie optique et vibrationnelle »**: 15-20 research groups involved with 5 already having a database in SSHADE.
- SSHADE: **thematic repository** for this field

➔ need a **simplified µ-SSDM data model** for simplified data + metadata import

- But we would like to have it ‘compatible’ with SSDM-Spectra for:
  - Common but adapted storage, import parser …
  - Common but reduced capabilities of the search / visualization / export / analysis tools
  - Possibility to upgrade metadata to SSDM-Spectra

# Numerous future ways to exploit SSDM & the SSHADE content

- SSDM and its content contain **numerous potentialities** partly exploited:
  - Publications database on solid spectroscopy:  600 publis
- Or not yet exploited, in particular thanks to its ‘fundamental bases’:
  - Search on minerals and their physical / optical properties:  300 minerals
    - Less minerals than Webmin or Mindat, but more efficient to search and more links
    - Raman (RRUFF),
  - Search on solids and their physical / optical properties: 325 solids
    - No database , only very specialized, like structure, X-rays, or general (Wikipedia) but difficult to search …
  - Search on Meteorites : 330 meteorites
    - Well structured properties, compared to Mineralogical bulletin
  - Search on molecules : 262 molecules
    - Possibility to search by bonds (500) or chemical function (120), or orther properties
    - Not available in the major molecule databases like PubChem, …

# Thanks to all those who contribute(d) to the development of SSDM, GhoSST, SSHADE-Spectra and SSHADE-Bandlist

- Pierre Volcke
- Damien Albert (*)
- Philippe Bollard
- Alexandre Garenne
- Lydie Bonal (*)
- The SSHADE Partner team
- Olivier Poch
- Manon Furrer
- Etienne Dode (*)
- Lucia Mandon (*)

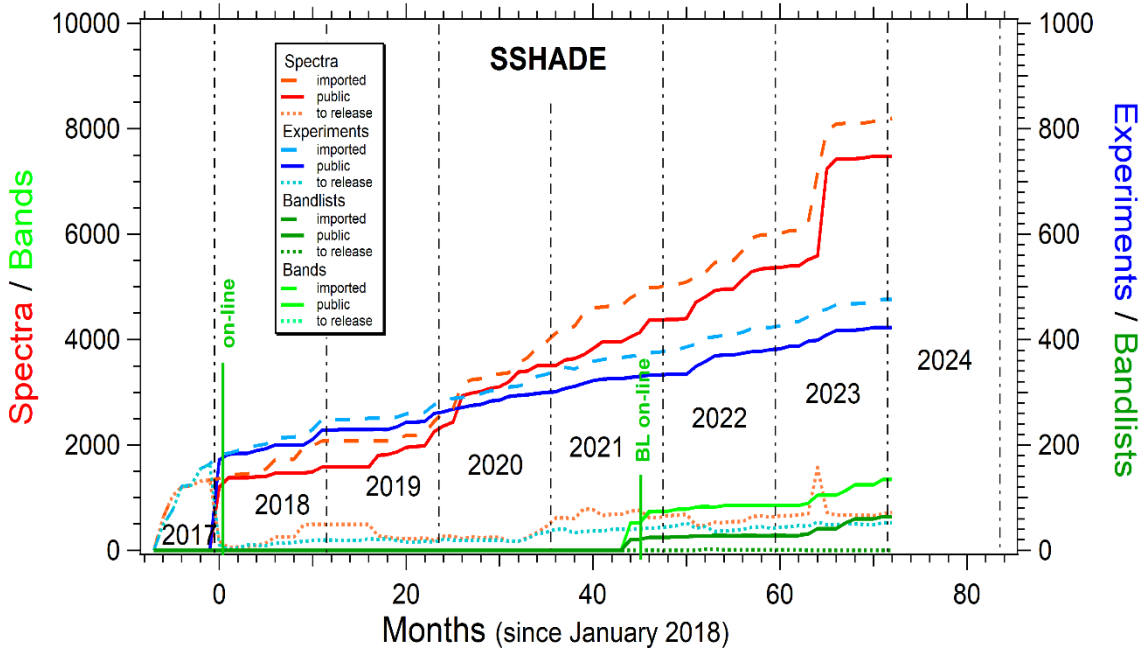
# The users of SSHADE

## Increasing content and use

- Today : 560 researchers registered users
- SSHADE data content

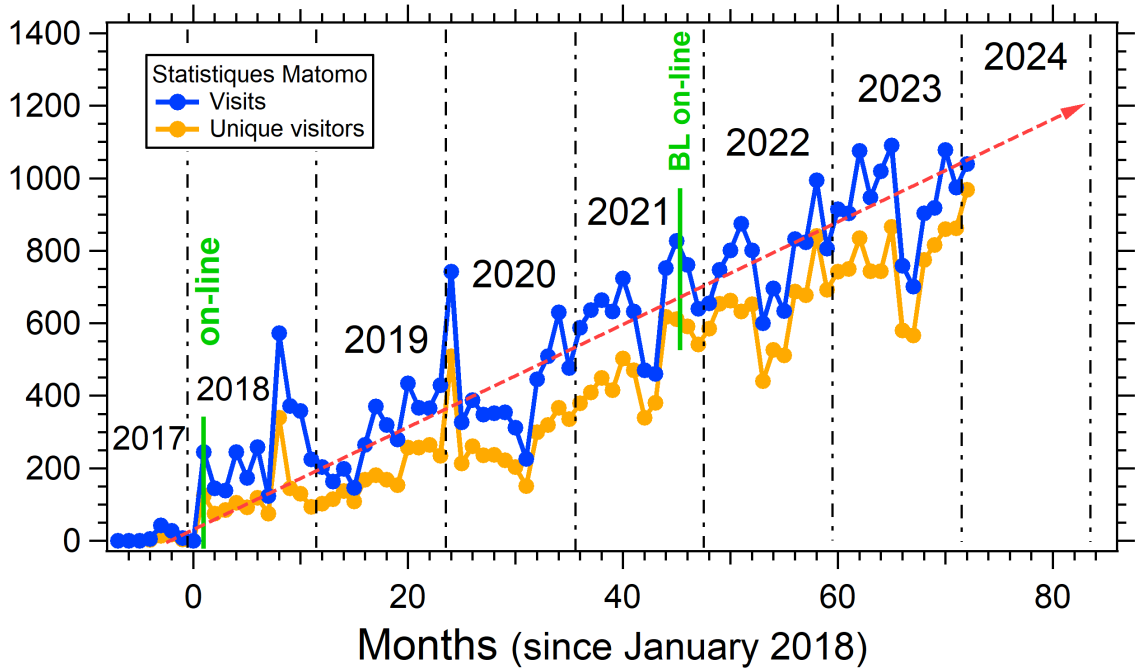
Experiments & Spectra & Bands

> 500 > 8200 > 1350




SSHADE users (Stats Matomo)

44% Europe, 31% USA+Canada, 22% Asia, 3% other



# Une longue histoire du dev de SSHADE

- Question : DM existant ou dev de SSDM ?
- Idée de départ: well structured and documented data, containing all necessary info (sample, instruments, spectra, …)
- Initial SSDM + demonstrateur SPIP ! 2005 ?
- Premiers dev en SQL LPG 2006-2008 (PV)
- Developpement de GhoSST Europlanet 2009-2012 (DA + PB)
  - Simple base surtout pour glaces, spectres trans, refl, kn…
  - But already in mind SSHADE
- Developpement de l'infrastructure SSHADE Europlanet-2020 RI (2015-2020) (PB + DA + AG + LB)
  - Data providers + independent databases, …
  - Extension des types de solides, types de spectres
  - Dev de meteorites, … données BRDF, XANES, …
- Developpement des listes de bandes (Ram+abs) @ SSHADE Europlanet-2024 RI (DA + MF)
  - + Dev de planetary objets + bodies
- Futurs dev
  - User data, user groups
  - New types of spectra: grains scattering, spectro-photo polarimetry (grains, surfaces), fluo matrix (vs excitation wavelength)
  - Bandlist: Bands parameters functions (T, P, …), molecular parameters
  - Reduced SSDM for RéGEF, …

  - Tracer nb pages SSDM = f(t)