

# Last developments of **GhoSST** and its **Solid Spectroscopy Data Model**

## The **SSHADÉ** project



Bernard Schmitt, Damien Albert, Philippe Bollard, Lydie Bonal, Maria Gorbacheva, P. Beck, E. Quirico and the SSDM Expert group\*

Institut de Planétologie et Astrophysique de Grenoble, CNRS / UJF

Gho **SS** DM  
T  
HADE



## Solid Spectroscopy Data Bases

**SSDM:** *the Data Model*

**SSHADE:** *the Hosting Architecture of Databases*

**GhoSST:** *the first Database in Grenoble for Astrophysics and Planetology*

## European projects: *IDIS/Europlanet* & *VAMDC* (2009-2012)

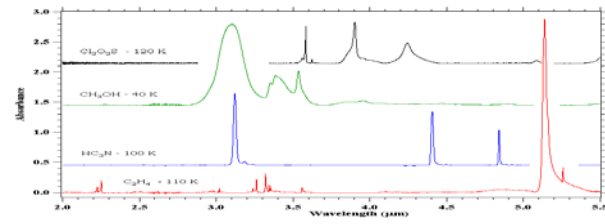
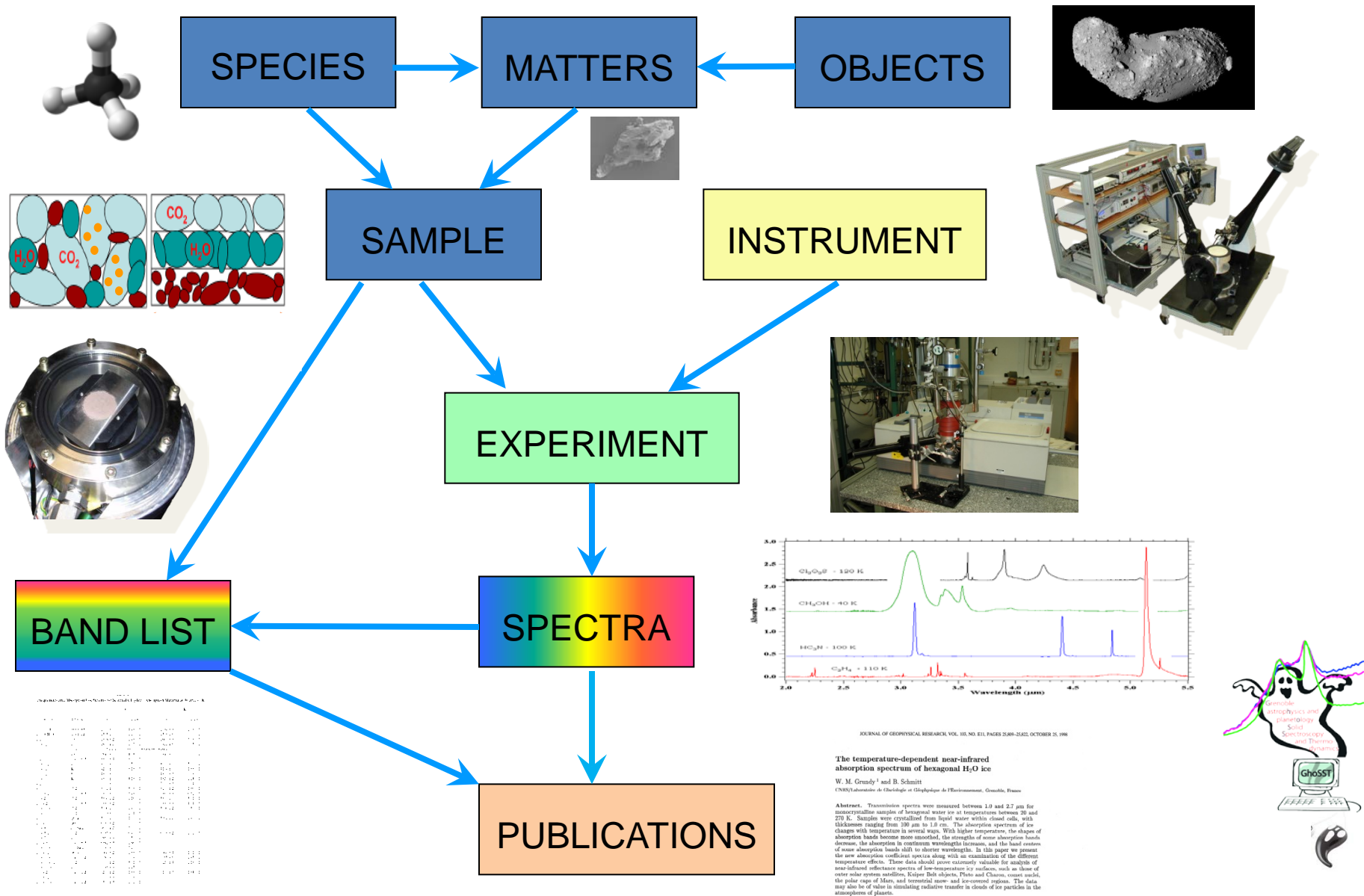
### Laboratory spectroscopic databases for solids :

- **Develop a Solid spectroscopy data model (SSDM)**
- **Generate a first new database with IPAG data (GhoSST)** covering :
  - UV-to-FIR transmission spectroscopy of ices and simple organics
  - UV-to-NIR bidirectional reflection spectroscopy of solid surfaces (planetary materials; minerals and ices, meteorites, organics, adsorption, processed, ...)
  - IR, Raman and Fluorescence micro-spectrometry  
(minerals, meteorites, organics...)
  - Band list of molecular solids and adsorbed molecules

→ **public version of GhoSST delivered: 25<sup>th</sup> September 2012**

- **Develop a generic database infrastructure (SSHADE)** (+ some tools)  
for spectroscopic data of solids *(to be available to other data producers, in a second step).*

# SSDM General Structure



JOURNAL OF GEOPHYSICAL RESEARCH, VOL. 103, NO. E11, PAGES 2389-2392, 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 Chimie et de 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 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 near infrared reflectance spectra of low-temperature ice samples, with an illustration of 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, comets 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.



# Development of SSDM Datamodel

(v 0.6)

\* **Improvements of core Data Model** (species/samples/instruments/spectra)

\* **Species and Matters:**

- **Mineral species**
- **Chemical functions**
- **Mineral & Rock matters**
- **Meteorite matters & meteorite objects**
- **Organic matters**

\* **Publications**

\* **Band list data model : bands and states**

- Bands parameters
  - position (energy), width, shape, intensities (peak and integrated)
  - accuracy / quality / evaluation
- Transitions assignment
  - states QN, ...

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# Minerals

Home Search Data Producer Manager User



Data / Publication / Mineral

Mineral Constituents

## Mineral

ID 58  
Type silicate

## Names

IMA Name Montmorillonite

## Chemical composition

Formula  $(Na, Ca)_{0.3}(Al, Mg)_2Si_4O_{10}(OH)_2 \cdot n(H_2O)$   
 Hydration Yes  
 Hydration series Yes  
 Hydration number n  
 Hydration number range 0 - n  
 Solid solution series variable mineral  
 Chemical formula  $(Na, Ca)_{0.3}(Al, Mg)_2Si_4O_{10}(OH)_2 \cdot n(H_2O)$   
 Chemical functions number 2  
 Chemical functions

~75 imported

Show 10 entries Search:

ID	UID	Type	Number	Common name	IUPAC name	Stoichiometric formula
227	SMOLEC_HOH	small molecule		HOH bond	HOH bond	H2O
253	IONRAD_OH	anionic radical		Hydroxide anion	Hydroxide anion	OH-1

Showing 1 to 2 of 2 entries

## Atomic composition

Elemental formula  $(Na)_x(Ca)_x(Al)_x(Mg)_xSi_4O_{12}H_2$   
 Atoms number 7  
 Atoms

Show 10 entries Search:

ID	UID	Symbol	Name	IUPAC name	Atomic number Z	Inchi
82	ATOM_H	H	Hydrogen	Hydrogen	1	1S/H
98	ATOM_O	O	Oxygen	Oxygen	8	1S/O
107	ATOM_Na	Na	Sodium	Sodium	11	1S/Na
108	ATOM_Mg	Mg	Magnesium	Magnesium	12	1S/Mg
109	ATOM_Al	Al	Aluminium	Aluminium	13	1S/Al
110	ATOM_Si	Si	Silicon	Silicon	14	1S/Si
129	ATOM_Ca	Ca	Calcium	Calcium	20	1S/Ca

## Oxides composition

Oxides

Show 10 entries Search:

Formula	Mass fraction
Al2O3	0
CaO	0
H2O	0
MgO	0
Na2O	0
SiO2	0

Showing 1 to 6 of 6 entries

## Classification

Strunz class silicates (09)  
 Strunz division phyllosilicate (09.E)  
 Strunz family Phyllosilicates with mica sheets, composed of tetrahedral and octahedral nets (09.EC)  
 Strunz code 09.EC.40  
 Dana major class Silicates (VIII)  
 Dana class phyllosilicate sheets of six-membered rings (71)  
 Dana type with 2:1 clays (71.03)  
 Dana group Smectite group (Diocahedral Smectites) (71.03.01a)  
 Dana code 71.03.01a.02

## Crystallography

Crystal system monoclinic  
 Crystal class prismatic  
 Crystal class symbol 2/m (C2h)  
 Space group C2/m

## Properties

Molar mass 549.07  
 Density 2.35  
 Density range 2 - 2.7

## Optical properties

Refringence type biaxial  
 Birefringence 0.0175  
 Birefringence range 0.0150 - 0.0200  
 Refringence sign negatif  
 Indexes na 1.51  
 Indexes na ranges 1.485 - 1.535  
 Indexes nb 1.527  
 Indexes nb ranges 1.504 - 1.550  
 Indexes ng 1.527  
 Indexes ng ranges 1.505 - 1.550  
 Dispersion V range none

## Optical aspect

Pure color white  
 True color gray white, yellow, brownish yellow, greenish

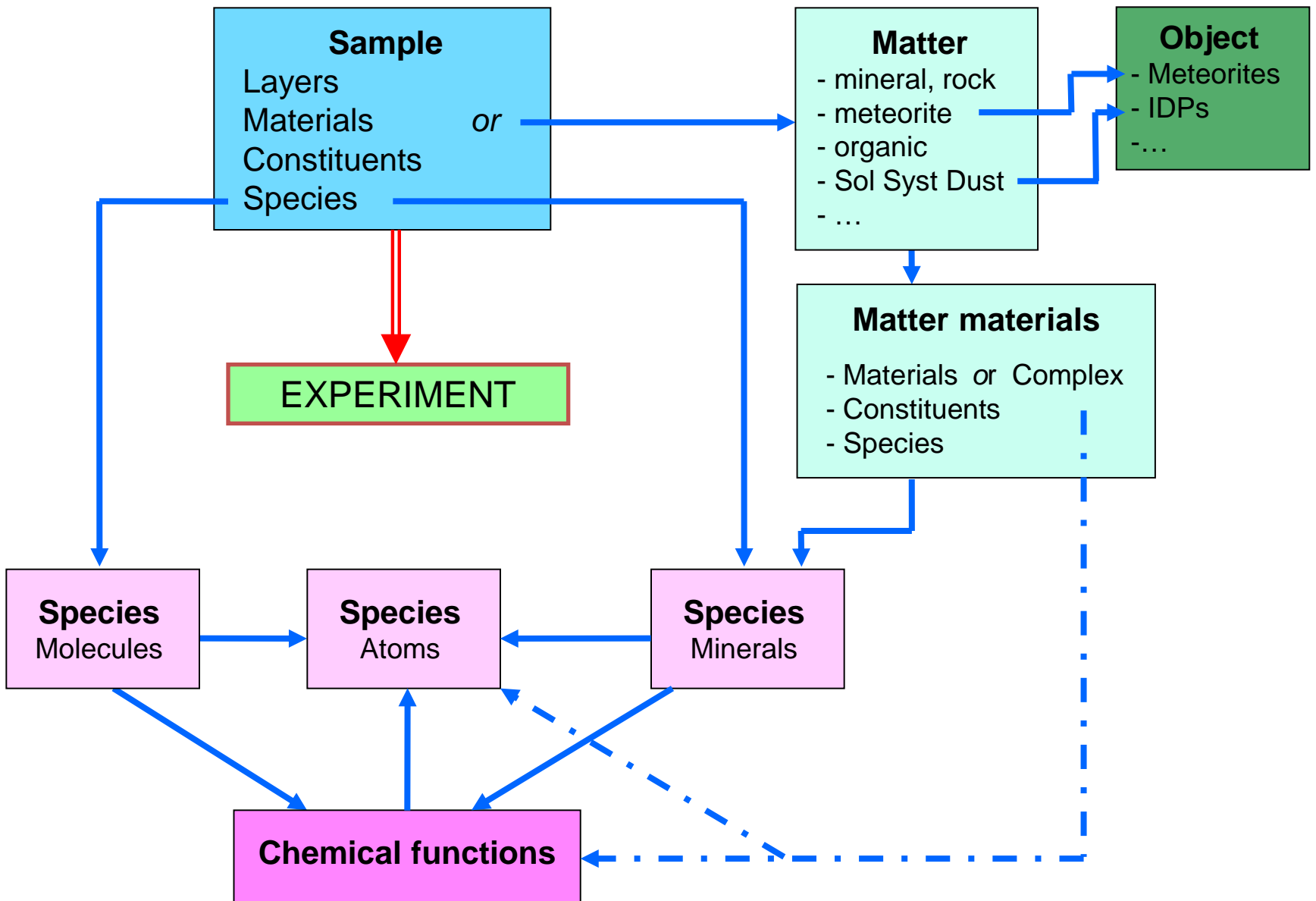
# Development of SSDM Datamodel

(v 0.6)

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# Sample – Species – Matters & Objects



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# Publications

## Publication

ID	104
UID	PUBLI_Schmitt_2003
Authors	<b>B. Schmitt</b> , S. Rodriguez
Year	<b>2003</b>
Title	Possible identification of local deposits of Cl <sub>2</sub> SO <sub>2</sub> on Io from NIMS/Galileo spectra

77 imported

## Type and access

Type	journal
Document type	article
State	published
Access rights	publisher free

## Content

**Abstract**

Starting from the recent discovery of chlorine ions in Io's plasma torus, we searched for evidence of Cl-bearing species at the surface of the satellite. We have identified Cl<sub>2</sub>SO<sub>2</sub>, with possible contribution by ClSO<sub>2</sub>, as candidates for the absorber(s) of the 3.92 μm band locally present in NIMS/Galileo spectra of the reddish deposits south of Marduk's volcanic center. Low-temperature laboratory measurements of the infrared spectra of several Cl and S-bearing molecules in the solid state, coupled with radiative transfer modeling, first allowed us to select four candidate molecules. Their abundance and stability at Io's surface have been tested through formation, condensation, and destruction scenarios using volcanic and atmospheric models completed with chemical and thermodynamical data. In particular, the sublimation rates of solid Cl<sub>2</sub>SO<sub>2</sub> and SO<sub>2</sub> have been measured to study the selective condensation of these species. Cl<sub>2</sub>SO<sub>2</sub> diluted at ~1% in a millimeter thick layer of solid SO<sub>2</sub> is the favorite candidate for the 3.92 μm band. We strongly favor a formation process of this molecule by heterogeneous reaction of Cl atoms on SO<sub>2</sub> ice condensing on plume particles or at Io's surface. The high Cl<sub>2</sub>SO<sub>2</sub> abundance observed implies that a Cl-rich volcanic eruption ( $[Cl - (Na + K)]/S > 0.015$ ) occurred at Marduk. ClSO<sub>2</sub> is a potential additional contributor to the band. Pure H<sub>2</sub>S is safely discarded as it is extremely unstable at Io's surface but an upper limit of 0.01% is derived for H<sub>2</sub>S diluted in SO<sub>2</sub>. Finally, chemical constraints allow us to firmly exclude H<sub>2</sub>S<sub>2</sub>. We also suggest that Cl<sub>2</sub>S may be an alternative explanation for the reddish coloration of some volcanic deposits.

**Keywords** spectroscopy, thermodynamics, transmission, absorbance spectra, optical constants spectra, band position, near-IR, molecular solid, ice, Cl<sub>2</sub>SO<sub>2</sub>, SO<sub>2</sub>, H<sub>2</sub>S, radiative transfer simulation, surface, Io

**Contents** sample, spectral data, thermodynamic data, planetary sciences, spectral data use,

## Document

Journal	Journal of Geophysical Research - Planets
Acronym	JGR E
Volume	108
Issue	E9
First page	5104
Last page	5122
Pages number	19

## Links

Pdf	<a href="#">schmitt03-JGRE-108-5104.pdf</a>
Doi	<a href="#">10.1029/2002JE001988</a>
Url	<a href="http://dx.doi.org/10.1029/2002JE001988">http://dx.doi.org/10.1029/2002JE001988</a>
ADS Url	<a href="http://adsabs.harvard.edu/abs/2003JGRE...108.5104S">http://adsabs.harvard.edu/abs/2003JGRE...108.5104S</a>

# Development of SSDM Datamodel

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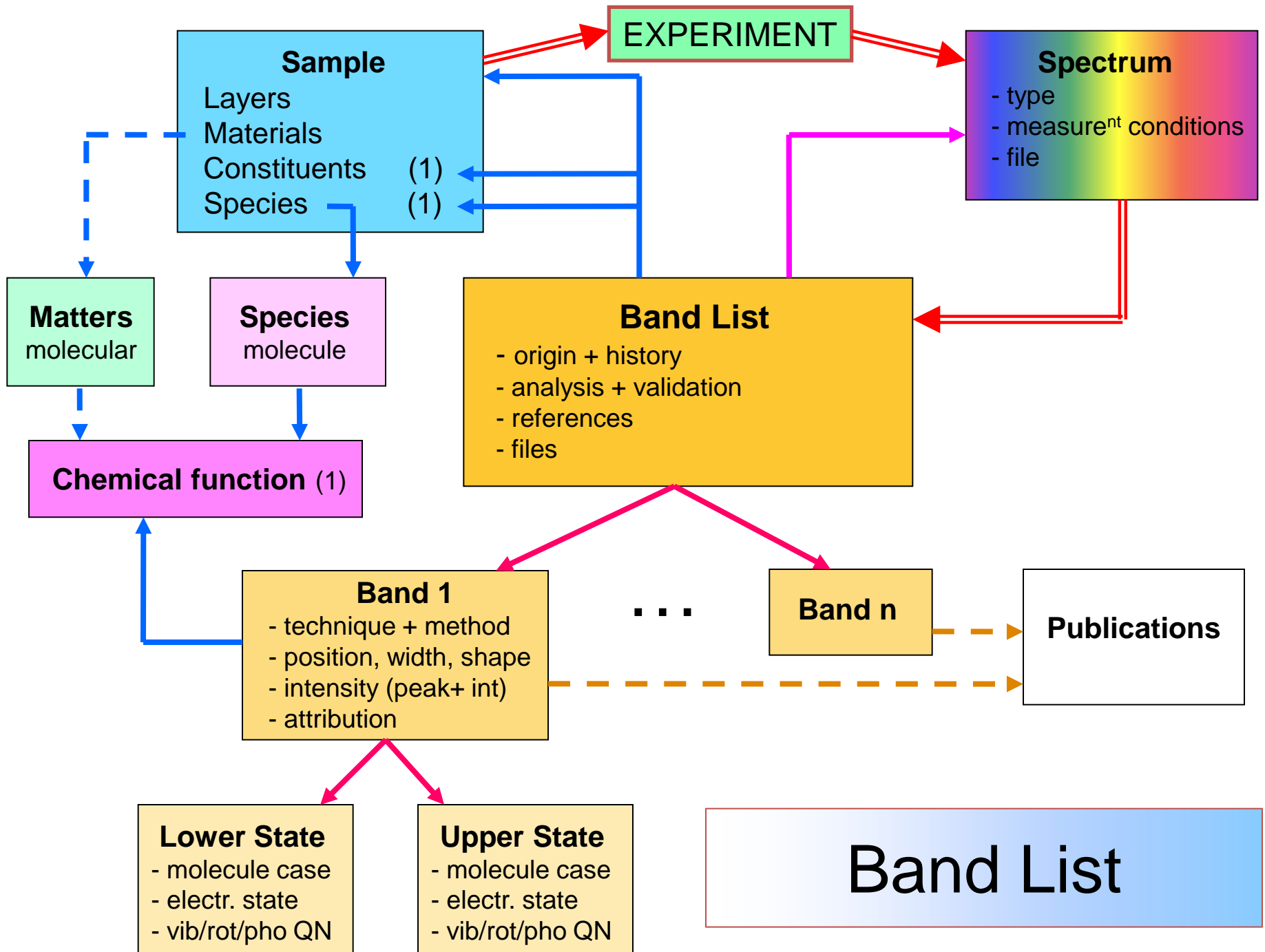
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# Band list and Bands

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

10 imported

Show 10 entries Search:

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

Showing 1 to 2 of 2 entries

**References**  
Publication state published

**Files**  
Filename bandlist\_12CH4-pureCH4iceI-30K-NIR  
Original filename CH4-freq-table\_Grundy02.png

Documentation • Contact • History • Credits • Statistics

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

# Development of GhoSST interface

import / search / visualization / export / ... : still lot of developments in progress

GhoSST
Data / Experiment / Sample / Layer

**Layer**

ID 47

**Layer organization in sample**

Order 1

Type granular

Comments small mechanical pressure when sample was flattened with a spatula

**Layer physical characteristics**

Thickness (mm) 1

Thickness error (mm) 0.1

Texture loose granular

Porosity 0.53

Density (g/cm3) 0.65

**Layer formation conditions**

Deposition conditions manual deposition

Deposition temperature (K) 300

Annealing temperature (K) 443

**Layer materials mixing**

Number of materials 4

**Sample**

**Sample name and references**

ID 48

Sample name H2O adsorbed on Smectite - 243K

Date 2008-02-01

Comments Sample temperature error is mostly due to possible vertical temperature gradient in the sample. Temperature reading accuracy and stability is 0.1K - Fluid error depicts estimated thermal cell - H2O saturation pressure at 243K is 0.37mb

**Sample physical characteristics**

Surface roughness low

Thickness 1 mm

**Sample layers organization**

Number of layers 1

Layer addition The sample holder is filled to rim with the non-compacted sample powder and then flattened with a spatula to obtain a smooth surface with limited powder compaction

**Sample substrate**

Substrate material aluminum anodized black

**Sample processings**

Processing type fluid

Temperature (K) 243.1

Annealing temperature (K) 443

Pressure (bar) 0

[More details...](#)

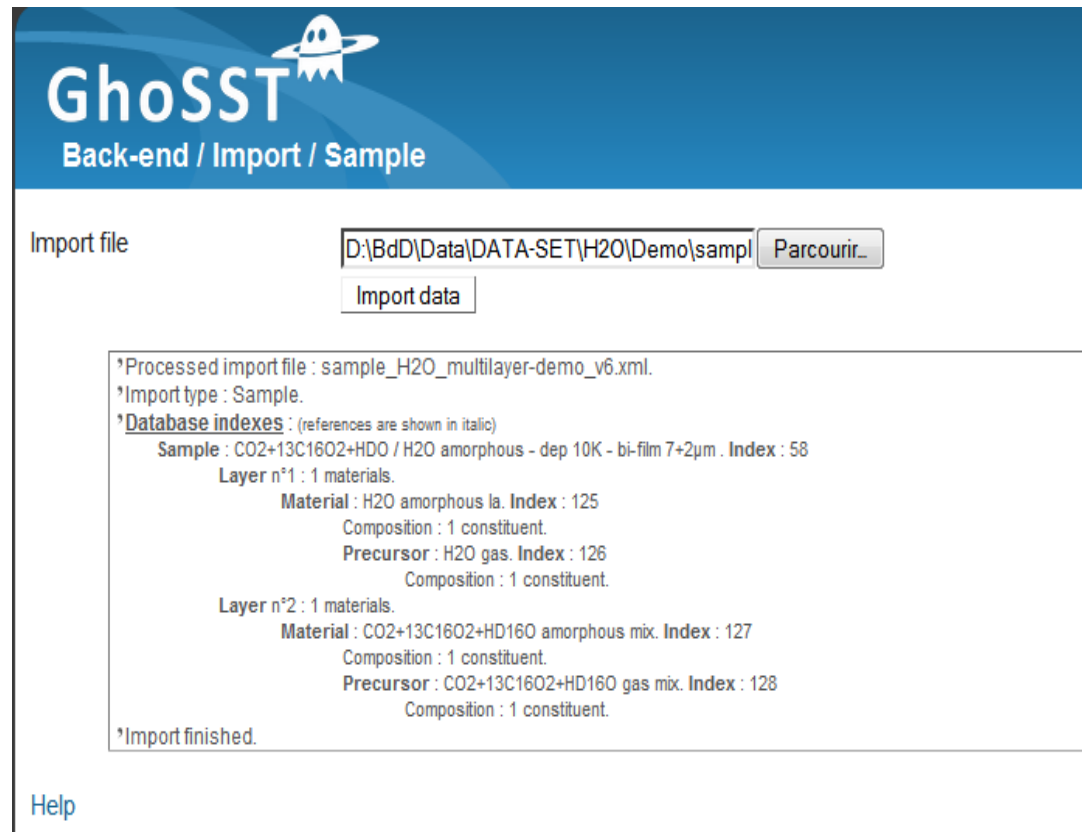
**Materials**

Actions	ID	Name	Matter origin	Matter family	Mole fraction	Mass fraction
<a href="#">View</a>	85	Smectite with adsorbed H2O	terrestrial	mineral		0.75
<a href="#">View</a>	86	Quartz	terrestrial	mineral		0.08
<a href="#">View</a>	87	Feldspar	terrestrial	mineral		0.16
<a href="#">View</a>	88	Gypsum	terrestrial	mineral		0.01

# IMPORT for DATA PRODUCERS

## Developed:

- xml templates for each data type
- import tools + validators
- control interface
- import history
- import documentation
- import tutorials



The screenshot shows the GhosST software interface. At the top, there is a blue header with the GhosST logo (a ghost with a ring) and the text "GhosST Back-end / Import / Sample". Below the header, there is a section for "Import file" with a text input field containing the path "D:\BdD\Data\DATA-SET\H2O\Demo\samp" and a "Parcourir..." button. Below the input field is an "Import data" button. A large text area below displays the following information:

```
*Processed import file : sample_H2O_multilayer-demo_v6.xml.  
*Import type : Sample.  
*Database indexes : (references are shown in italic)  
  Sample : CO2+13C16O2+HDO / H2O amorphous - dep 10K - bi-film 7+2µm . Index : 58  
    Layer n°1 : 1 materials.  
      Material : H2O amorphous la. Index : 125  
        Composition : 1 constituent.  
        Precursor : H2O gas. Index : 126  
          Composition : 1 constituent.  
    Layer n°2 : 1 materials.  
      Material : CO2+13C16O2+HD16O amorphous mix. Index : 127  
        Composition : 1 constituent.  
        Precursor : CO2+13C16O2+HD16O gas mix. Index : 128  
          Composition : 1 constituent.  
*Import finished.
```

At the bottom left of the interface, there is a "Help" link.

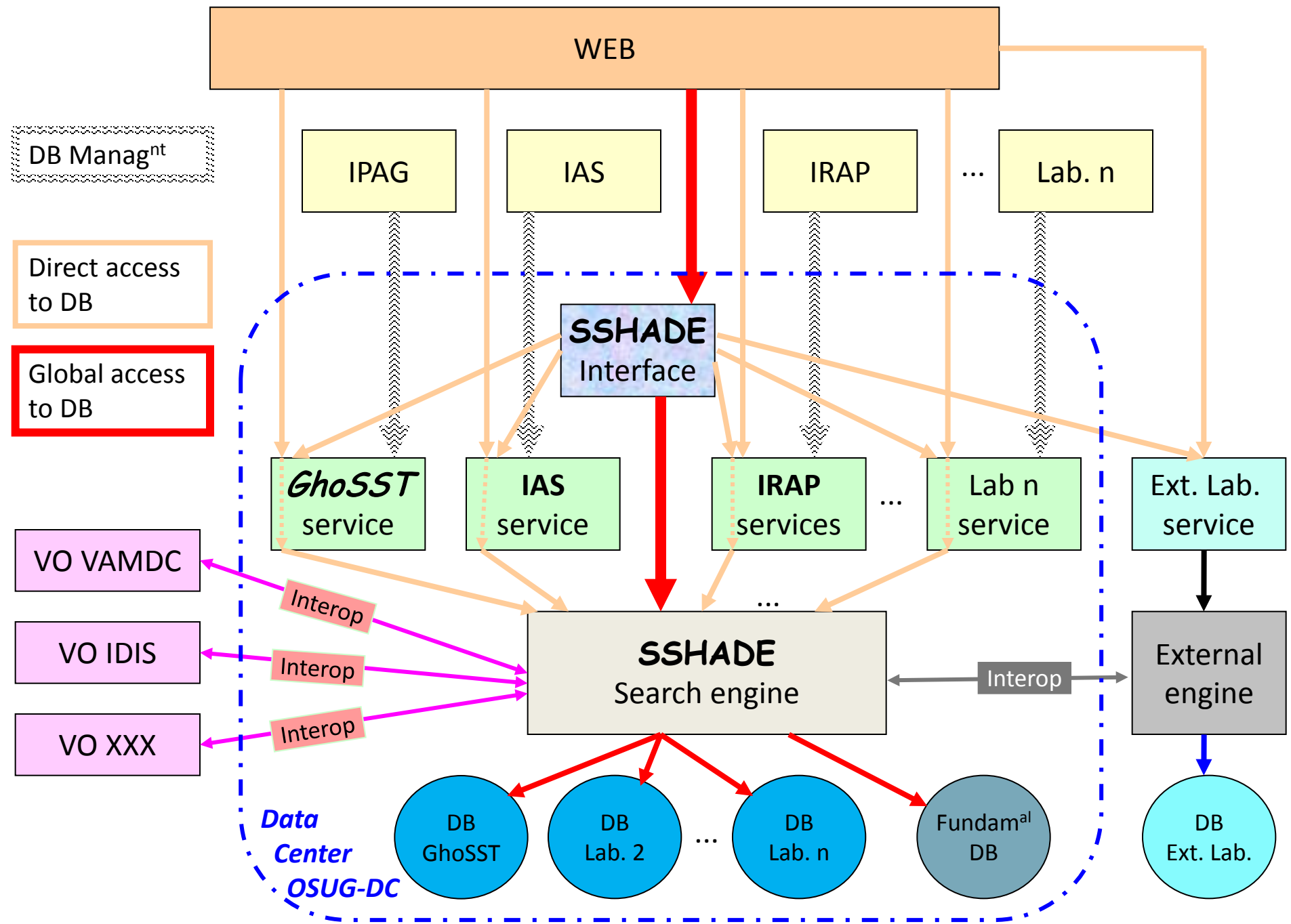


# Hosting Solid Spectroscopy data of other Data Providers: *SSHADÉ*

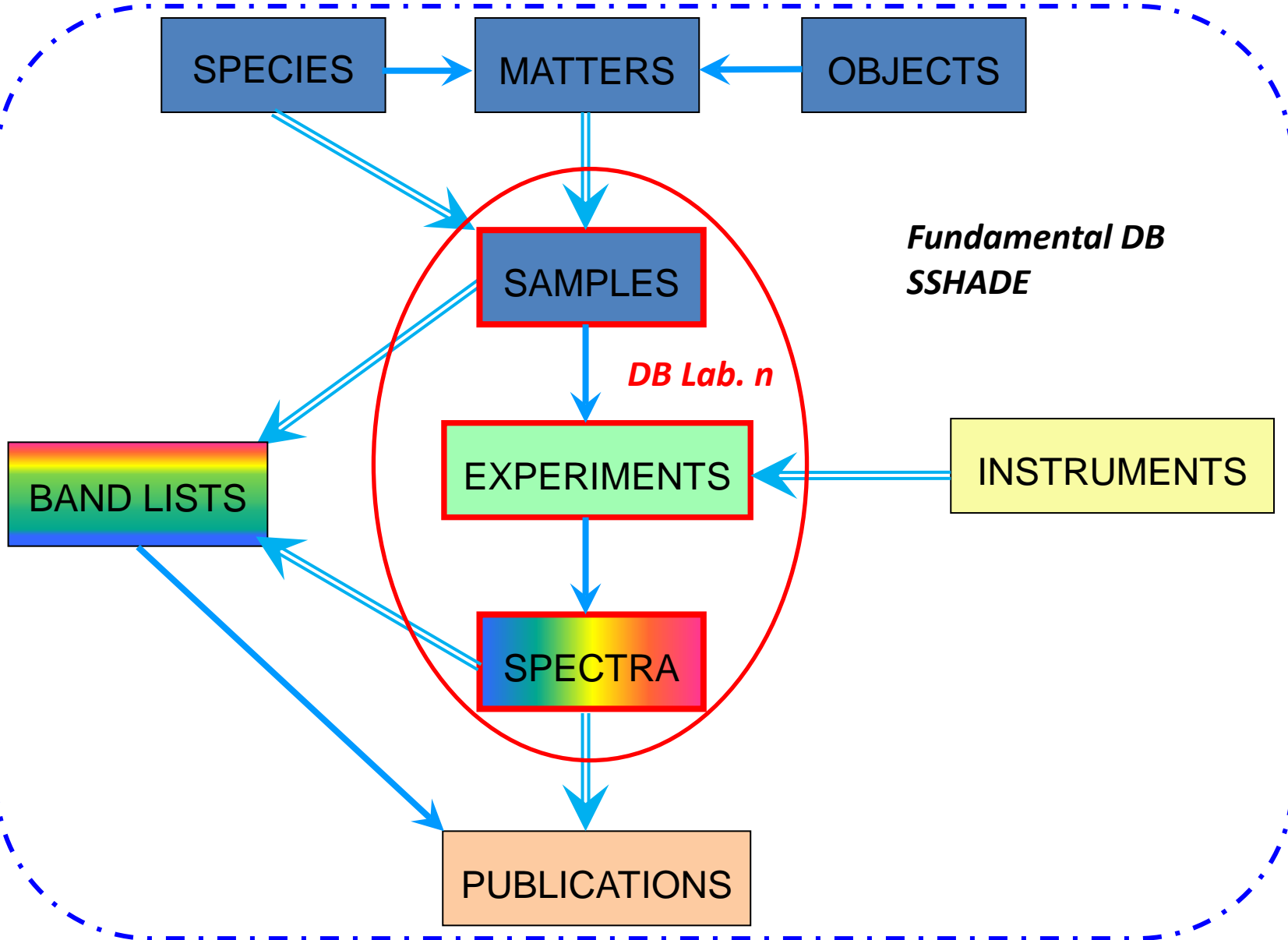
***SSHADÉ*** :

***“Solid Spectroscopy Hosting Architecture of Databases and Expertise”***

- Solid Spectroscopy interface
- A database per laboratory
- Also direct link to each individual DB interfaces
- All databases and engines hosted at OSUG data center (OSU Grenoble - UJF)
- SSHADÉ will be a client of others VO (IDIS, VAMDC, ...)
- Possible to link to other external Solid Spect. databases (need interoperability layer with SSDM)



# SSHADE: new SSDM Structure



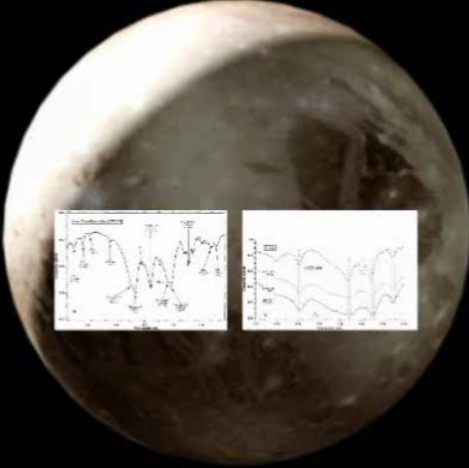
# SSHADÉ Project

- **VAMDC/EPN (2009-2012)**
  - Development of SSDM and GhoSST (with SSHADÉ compatibility in head)
  - Test of data ingestion by others laboratories
- **In progress:**
  - 2012: proposition of SSHADÉ to INSU/CNRS w. 5 French laboratories
  - 2013: GhoSST get label from INSU/CNRS  
Recommendation from INSU/CNRS to develop SSHADÉ  
Funding asked on French side (OSUG, INSU/CNRS, ASOV, CNES)
  - 10/2013: 1<sup>st</sup> meeting of SSHADÉ-France (IPAG, Grenoble)
  - 11/2013: 1<sup>st</sup> meeting of SSHADÉ-Europe (OU, Milton Keynes)
- **Project:**
  - **2014: start development of SSHADÉ infrastructure**
  - **2014/15: start 2-3 new DataBases** (to be selected)
  - European funding: *Horizon 2020* call ?

# look at Video: « GhoSST user case »

Pluto\_en

## Analyzing Pluto's surface



**About Pluto**

**First step: methane data relevant to Pluto**

**Second step: dinitrogen data relevant to Pluto**

**GhoSST<sup>+</sup>**  
SSW and GhoSST development:  
Bernard Schmitt: Scientific manager  
Guillaume Bibrac: Software manager  
Philippe Bédou: Software development  
Cristina Carro: Software development  
Lydie Bonel: Scientific development  
In order: contributors (data reduction and documentation)  
Alexander Krumm  
Alexandre Poncelet  
Marie-Catherine  
Pierre-André  
Benoît Quirion

**GhoSST<sup>+</sup>**  
**Thank you!**  
Other software used available on this computer:  
- Flighting computer  
- Thermal Database  
- Tracking algorithm  
- Subroutines: AMCA, LARIS, Tera  
- Analyzing Pluto's surface

## Using GhoSST

00:32