1st SSHADE partners meeting

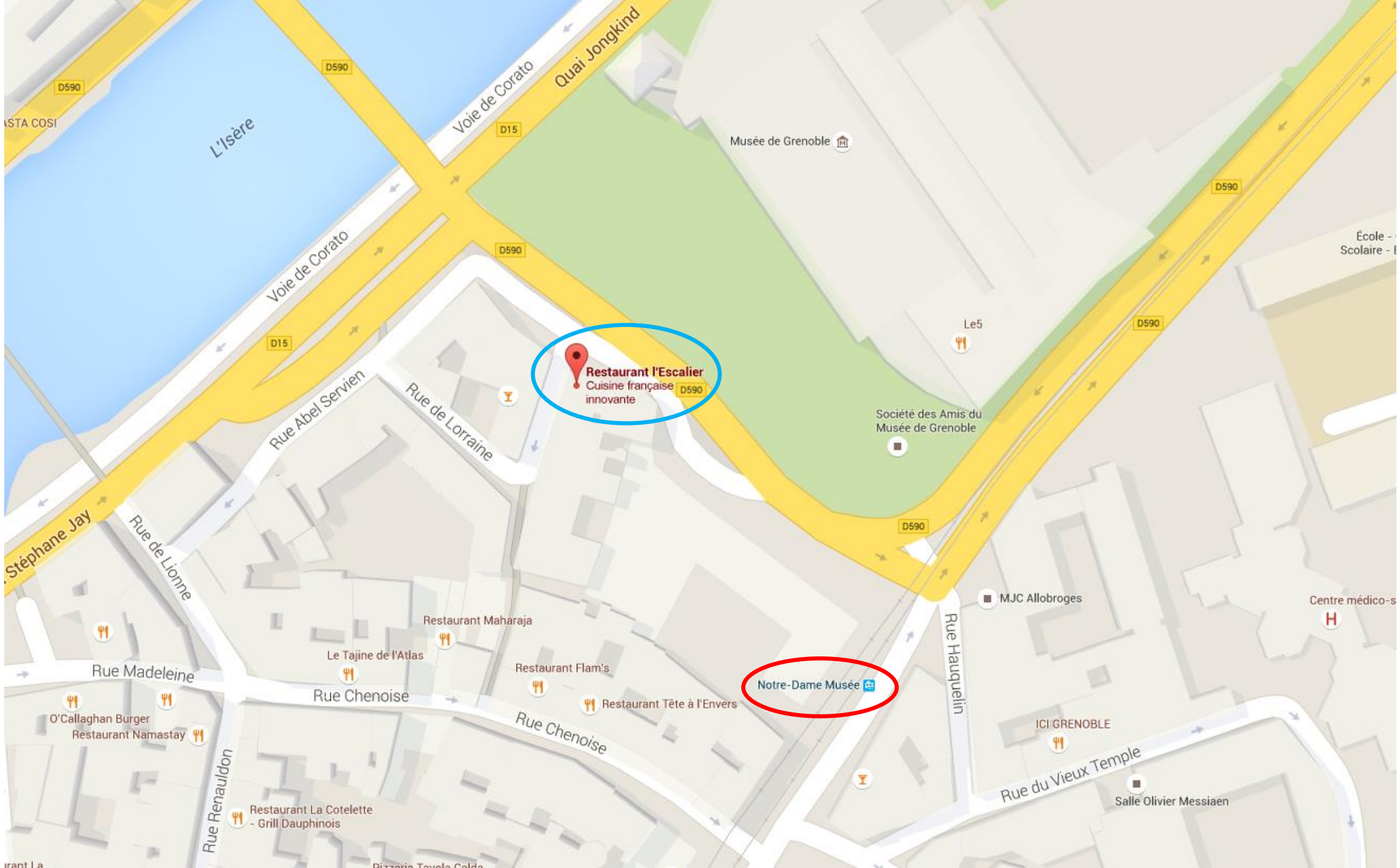
10-11 May 2016 – IPAG, Grenoble, France

Logistics

- Lunchs: will be taken at ‘No Name’ restaurant (5 min from here)

- Dinner Tuesday 10th 19:30 @ **restaurant « l’escalier »**
  6 place de Lavalette
  Tram B stop : « Notre-Dame Musée »

- Wednesday we start at 9:30
  but 3ème étage (4th floor) OSUG-D
  Room Oisans (300)


L'Isère
Quai Jongkind
Voie de Corato
D590
D15
Musée de Grenoble
Restaurant l'Escalier
Cuisine française innovante
Le5
Société des Amis du Musée de Grenoble
Rue Abel Servien
Rue de Lorraine
Rue de Lionne
Stéphane Jay
Rue Madeleine
Rue Chenoise
Restaurant Maharaja
Le Tajine de l'Atlas
Restaurant Flam's
Restaurant Tête à l'Envers
O'Callaghan Burger
Restaurant Namastay
Rue Renauldon
Restaurant La Cotelette - Grill Dauphinois
Notre-Dame Musée
Rue Hauquelin
MJC Allobroges
ICI GRENOBLE
Rue du Vieux Temple
Salle Olivier Messiaen
Centre médico-s
École - Scolaire

Aims of this 1st SSHADE partners meeting

To present:

- the project and the tasks to be realized during the 4 years of the Europlanet 2020-RI program.
- the current state of development of the SSHADE database infrastructure (JRA VESPA workpackage, task 3)
- its future developments.

To discuss:

- about organization of managers formation
- partner's database filling (VA VESPA workpackage, task 2)
- any question related to SSHADE.

A little bit of history: from past to future

- 2002: Idea ...
- 2006: Concept ...
  Content demonstrator: STSP
- 2007-2008: First “solid spectroscopy” datamodel
  Development of 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

✓ **4 Feb. 2014: GhoSST upgrade** (v0.6)

- 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 producers (VESPA VA)
SSHADE online (2017)

GhoSST Web interface

- Public version of GhoSST accessible at: http://ghosst.osug.fr

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SSHADE European Consortium of Data Providers

Consortium of **20** solid spectroscopy experimental groups
in **8** European countries (F, GB, D, I, E, CH, PL, HU)
involving ~**65** peoples

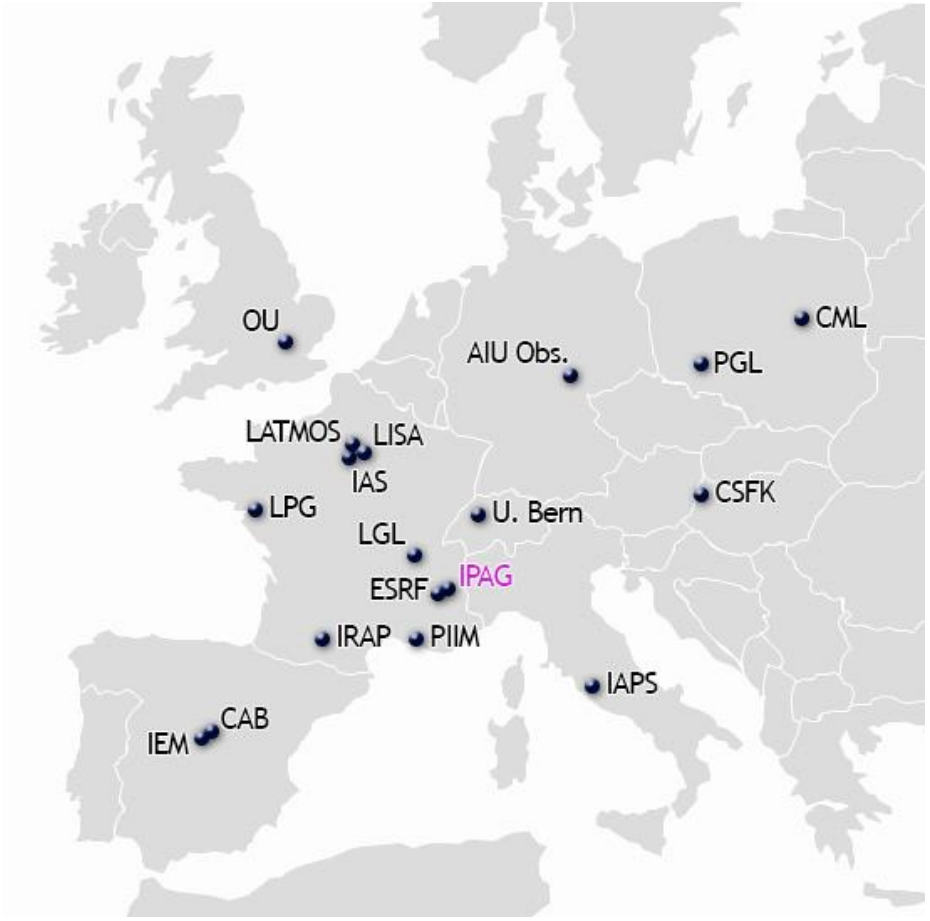
Each with particular expertises on:

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

SSHADE blog : http://blog.sshade.eu

The SSHADE-Europe consortium in EPN@2020-RI

- **IPAG / Planéto**, Grenoble - F (Bernard Schmitt, Lydie Bonal, Damien Albert)
- **Open University**, Milton Keynes – UK (Nigel Mason)
- **IAS**, Univ. Paris-Sud - F (Emmanuel Dartois, Donia Baklouti)
- **IRAP / GPPS**, Toulouse - F (Patrick Pinet, Yves Daydou)
- **IRAP / MICMAC**, Toulouse - F (Karine Demyk , Yves Daydou)
- **LPG**, Univ. Nantes - F (Yann Morizet, Manuel Giraud)
- **Space and Planetary Science Division**, Univ. of Bern - CH (Antoine Pommerol)
- **PIIM**, Univ. Aix-Marseille - F (Patrice Theulé)
- **IAPS**, INAF, Roma - I (Alessandra Rotundi, Vincenzo della Corte)
- **IAPS**, INAF, Roma - I (Fabrizio Capaccioni, Christian Carli)
- **LISA,** Univ. Paris-Est - F (Nicolas Fray)
- **AIU Observatory**, Jena - D (Harald Mutschke, Jürgen Weiprecht) [DOCCD 'database']
- **Centro de Astrobiología**, INTA-CSIC – E (Guillermo Muñoz Caro)
- **Instituto de Estructura de la Materia**, Madrid – E (Vicente Timón, Miguel Angel Moreno)
- **LATMOS / IMPEC**, Institut Pierre Simon Laplace - F (Nathalie Carrasco)
- **LGL / ENS-Lyon** - F (Bruno Reynard, Gilles Montagnac (exp.), Razvan Caracas (theory)
- **Konkoly Astronomical Institute** – HU (Akos Kereszturi)
- **Planetary Geology Lab.**, Institute of Geological Sciences, Polish Academy of Sciences – PL (Joanna Gurgurewicz, Luigi Castaldo)
- **Clay Mineral Laboratory**, Institute of Geological Sciences, Polish Academy of Sciences – PL (Joanna Gurgurewicz, Luigi Castaldo)
- **ESRF / FAME line**, Grenoble – EU / F (Denis Testemale, Isabelle Kieffer)



Data of SSHADE

- **Spectral ranges:**
  - from X-ray to mm (through UV-Vis-IR)

- **Solids:**
  - Ices (low to high pressure, low to room temperature, mixtures, matrix isolated, ...)
  - clathrates hydrates, hydrates
  - minerals (naturals and synthesized), rocs
  - organic matter (natural and synthesized), polymers, VUV
  - Extraterrestrial matter: meteorites, IDPs, ...
  - also liquids

- **Data types:**

➢ **Spectra**
  - infrared transmission spectra, absorption coefficients, optical constants
  - Raman spectra et micro-spectroscopy
  - reflectance spectra of surfaces, spectro-photometric functions
  - multispectral and multi-angular imagery of surfaces

➢ **Bandlist**
  - position, width, intensity, attribution ... for molecular solids

SSHADE Solid Spectroscopy Data (1)

- **IPAG** ***(GhoSST)***
  - Vis-FIR spectra, optical constants and bandlists of ices, minerals/rocks, organic molecules and materials, optical materials.
  - Vis-NIR bidirectionnal reflectance spectra + BRDF of surfaces: snows, ices, minerals/rocks, organic materials, salts, sulfur, ...
  - UV-Vis Raman + Fluorescence spectra + Band parameters of organic molecules, natural et synthetic carbonaceous materials, meteorites, IDPs, Stardust grains.
  - NIR+MIR microscopic spectro-images of carbonaceous materials, minerals/rocks.
- **IAS**
  - MIR spectra of ices and clathrates hydrates
  - MIR spectra organic molecules and materials synthesized by VUV irradiation
  - MIR+FIR spectra of synthetic carbonaceous materials.
  - MIR+FIR spectra and Raman micro-spectroscopy of meteorites, IDPs, …
- **LPGNantes**
  - Raman spectra of ices and clathrates hydrates at high pressures
  - NIR reflectance spectra of ices, clathrates hydrates and minerals
- **IRAP-GPPS**
  - multispectral and multi-angular imagery of mineral surfaces
  - multispectral photometric fonctions
- **IRAP- MICMAC**
  - FIR+sub-mm spectra and absorption coefficients of synthetic silicates
- **LISA**
  - MIR spectra of ices and organic polymers

SSHADE Solid Spectroscopy Data (2)

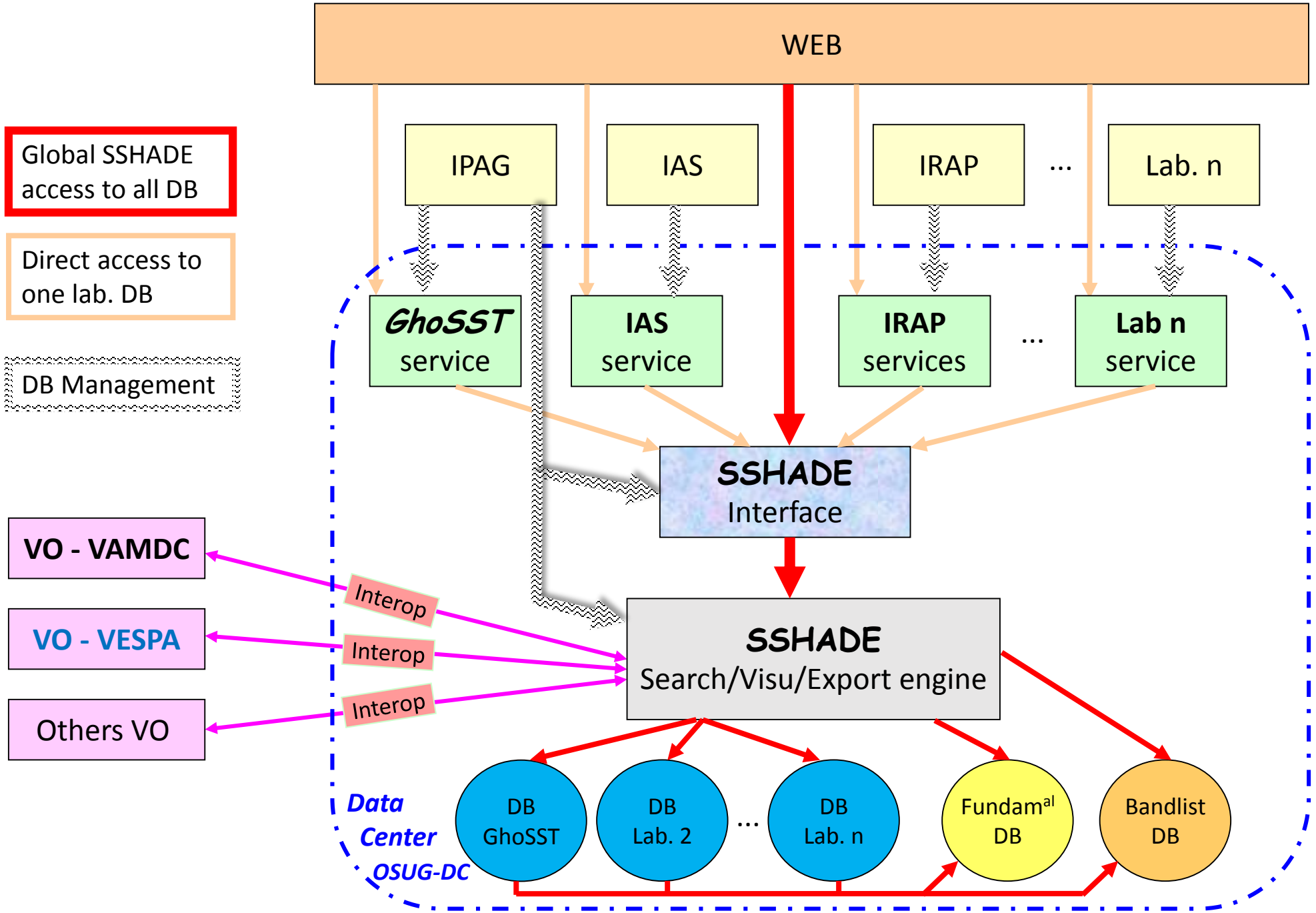
- **PIIM**
  - MIR spectra of ices and organic molecules synthesized by VUV irradiation and chemical reactions
  - MIR spectra de molecules isolated in matrices.
- **LATMOS**
  - MIR spectra of synthetic organics (tholins, ...)
- **LGL, ENS-Lyon**
  - Raman spectra of minerals and meteorites
- **Open University**
  - VUV spectra of ices
- **Catania Astrophysical Observatory**
  - MIR spectra of ices
- **IAPS**
  - Spectra of meteorites, minerals and rocks
- **Univ. of Bern**
  - multi-bands photometry of various materials: ices, organics, mixtures, ...
- **AIU Observatory** [DOCCD 'database']
  - optical constans of minerals
- **Centro de Astrobiología**
  - NIR-FIR spectra of ices ...
- **Instituto de Estructura de la Materia**
  - NIR-FIR spectra + optical constants of ices, organic molecules, phyllosilicates
- **Konkoly Astronomical Institute**
  - MIR spectra of meteorites and clay minerals

Solid Spectroscopy data Infrastructure for European Data Providers: *SSHADE*

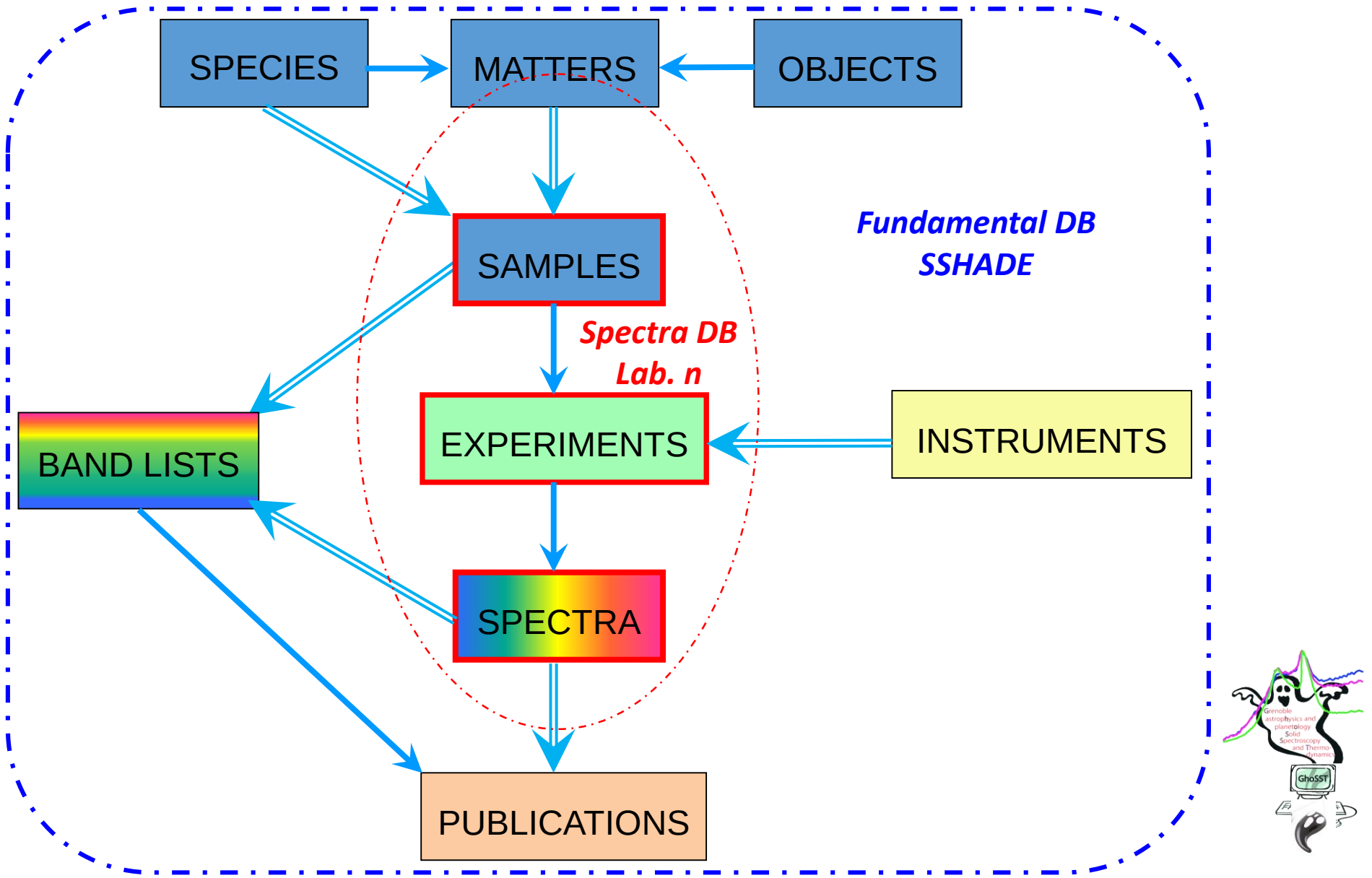
***SSHADE* :**

"Solid Spectroscopy Hosting Architecture of Databases and Expertise"

- Based on the ***GhoSST*** database developments (Europlanet + VAMDC)
  => http://ghosst.osug.fr
- Made of:
  - ✓ A 'solid spectroscopy' interface
  - ✓ A Search/Visualization/Export engine
  - ✓ A set of databases: one per group (GhoSST is one of them)
  - ✓ A common fundamental database
- All hosted at OSUG data center (OSU Grenoble – UGA *(formerly UJF)*)
- SSHADE will be a service of others VO (Europlanet-VO, VAMDC, ...)


WEB
Global SSHADE access to all DB
Direct access to one lab. DB
DB Management
IPAG
IAS
IRAP
...
Lab. n
GhoSST service
IAS service
IRAP services
...
Lab n service
SSHADE Interface
SSHADE Search/Visu/Export engine
VO - VAMDC
VO - VESPA
Others VO
Interop
Interop
Interop
DB GhoSST
DB Lab. 2
...
DB Lab. n
Fundamal DB
Bandlist DB
Data Center OSUG-DC

SSHADE: new SSDM Structure



Europlanet 2020-RI
JRA-5 Activities (WP 11)

JRA – SSHADE infrastructure development

Databases infrastructure (years 1 – 2)

- Adaptation of SSDM (data model)
- Reorganization of databases
- Rewriting data queries
- Design for easier data selection and browse
- Creation/customization of one database per Lab

Reorganization of databases

- Rewriting import parsers (year 1)
- Tools for easier data import (year 2)

VO interoperability

- with VESPA-VO and VAMDC-VO (years 2 – 3)

Europlanet 2020-RI
VA2 Activities (WP 6)

VAA – Database feeding

Coordination of consortium

- Animation of SSHADE consortium
- Preparation and feeding of the common fundamental data of SSHADE (Years 1 - 2)
- Development of the common 'band list database' (Years 2 - 4)

Support to consortium

- 3 SSHADE consortium meetings (Years 1, 2, 4)
- Formation/training of database managers and 'feeders' (Years 1 - 3)
- Preparation of documentations and tutorials for providers
- Technical support to adapt import file & interface to each data set
- In-situ & on-line support to each database manager
- Help feed data collected by the visitors of TNA on spectroscopic instruments

Support to users

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

Europlanet 2020-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 (2016-2019)**
  - **Micro-goniometre 'Gognito' for dark samples (2017-2019)**

Data

- Need to provide their data in open-access after 1 year
- Will be stored in a special database in SSHADE
- Will be set 'public' after one year.

Who do what ?

SSHADE management

- *Scientific Manager*: Bernard Schmitt (IPAG)
- *Software Manager*: Damien Albert (OSUG)

SSHADE development

- *Databases development*: Philippe Bollard (IPAG, formerly @ Coriolys)
- *Interfaces Design*: Maria Gorbacheva + Ph. B (Flex-Studia)
- *VO interoperability:* Damien Albert (OSUG)
- *Databases storage*: Damien Albert (OSUG Data Center, Grenoble)

Data bases feeding

- *Consortium/users support:* Alexandre Garenne + BS (scientific engineer @ IPAG)
- *Fundamental data feeding* Lydie Bonal + AG + BS (science team @ IPAG)
- *Data validation, DB animation* Scientific Managers (one at each consortium group)
- *Data preparation & import* Database Managers (one at each consortium group)

SSHADE Time line

2015

- September — **Start of Europlanet 2020-RI**
- November — Start of SSHADE development
- December — Training database managers (session #0)

2016

- May — 1st SSHADE meeting
- May — Training database managers (session #1) **(D6.3 VAA VESPA – Y1)**
- August — **SSHADE prototype delivery** **(D11.5 JRA VESPA)**
- November — Training database managers (session #2)

2017

- April — Training database managers (session #3)
- June — 3 databases ingested in SSHADE **(D6.3 VAA VESPA – Y2)**
- August — **SSHADE infrastructure** **(D11.7 JRA VESPA)**
- September — Training users EPSC (session #1) **(D6.5 VAA VESPA)**
- October — 6 databases ingested in SSHADE
- October — 2nd SSHADE meeting
- October — Training database managers (session #4)

SSHADE Time line

2018

- March — Training database managers (session #5)
- April — Training users EGU (session #2) — **(D6.5 VAA VESPA)**
- June — 9 databases ingested in SSHADE — **(D6.3 VAA VESPA – Y3)**
- September — Training users EPSC (session #3) — **(D6.5 VAA VESPA)**
- October — Training database managers (session #6)
- November — 12 databases ingested in SSHADE

2019

- March — 15 databases ingested in SSHADE
- March — 3rd SSHADE meeting
- April — Training users EGU (session #4) — **(D6.5 VAA VESPA)**
- June — 18 databases ingested in SSHADE
- August — **SSHADE with 18-20 databases** — **(D6.3 VAA VESPA – Y4)**
- August — **End of Europlanet 2020-RI**

Status of the preparation of fundamental data and plans

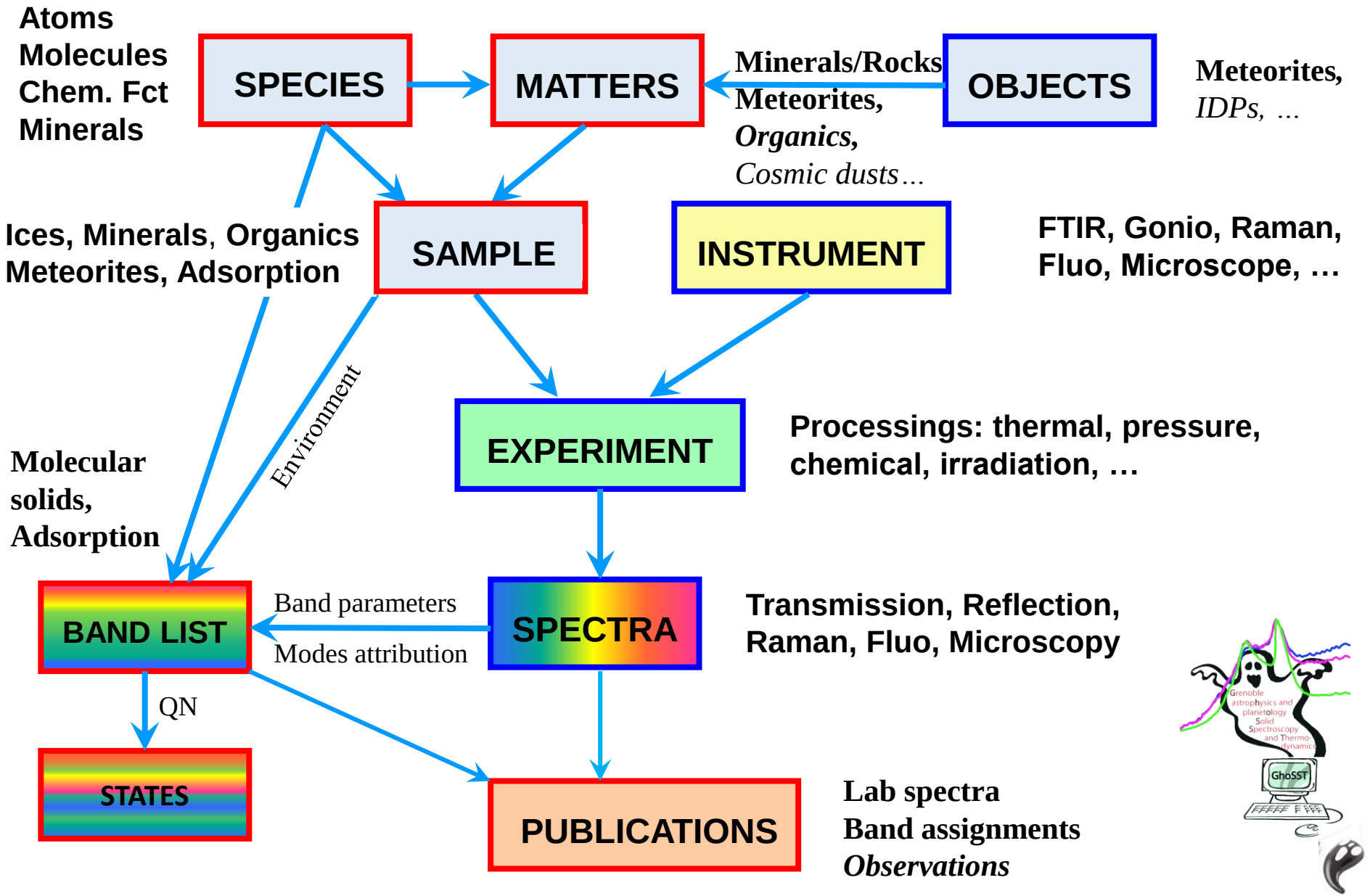
Fill and ingest in SSHADE the basic information necessary to build samples

- Species: Atoms, Chemical functions, Molecules, Minerals
- Matters: International standards, …
- Meteorite objects

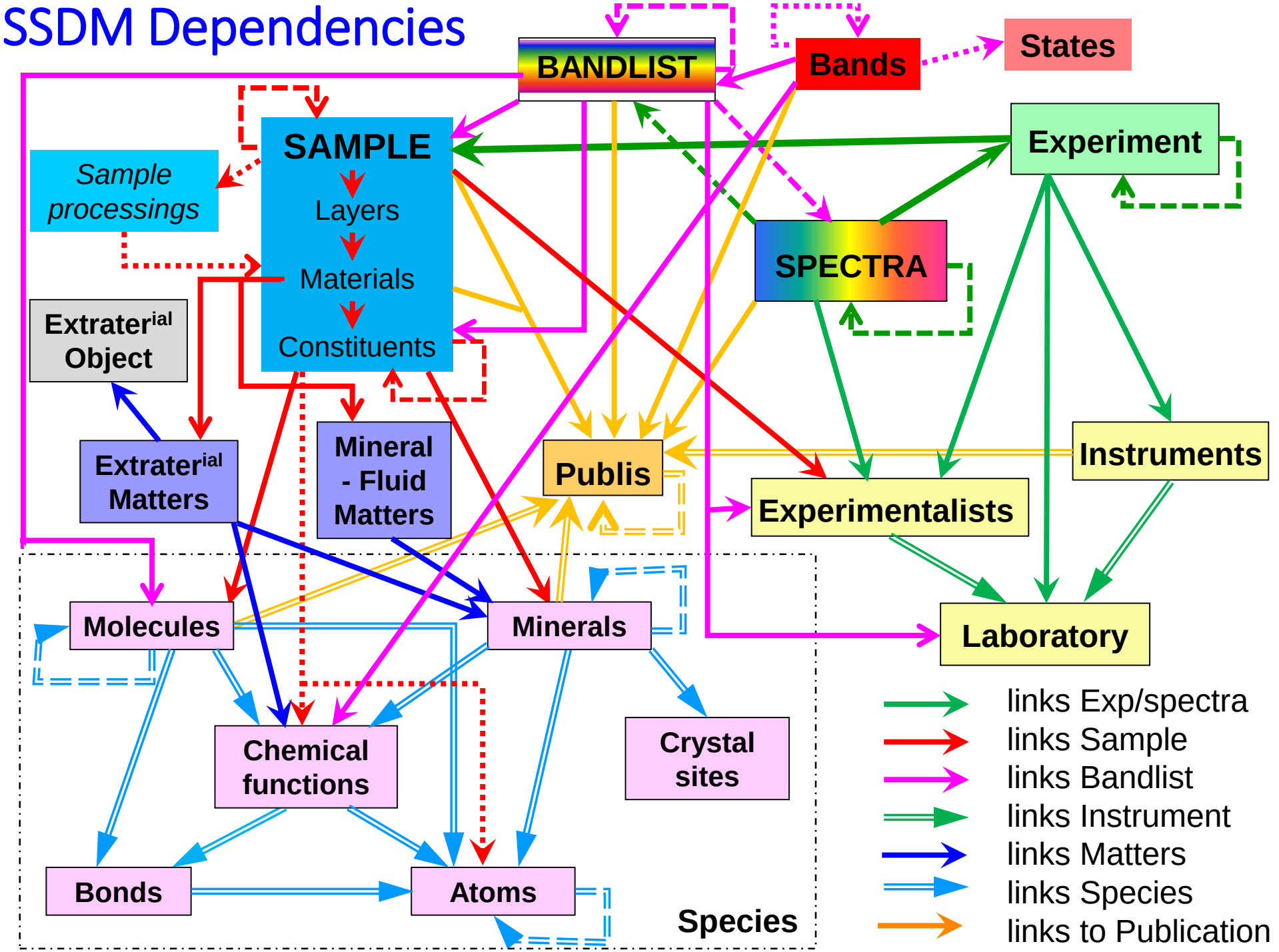
- Set up a bibliographic reference data base

- Band list of Molecular solids

SSDM General Structure



SSDM Dependencies



Status of the preparation of fundamental data and plans

Detailled information + links on:

- Atoms, bonds, Chemical functions (+ isotopes)
- Molecules (+ isotopic species)
- Minerals (+ series, sub-groups, groups)
- International standard matters (+ local matters)
- Meteorite objects

- **Publications of**
  - partners work (samples, spectra, insruments, techniques, …)
  - spectroscopy, standard matters, meteorite objects, …

- **Band list of Molecular solids**
  + associated publications

Molecule (1)

Molecule | Import history

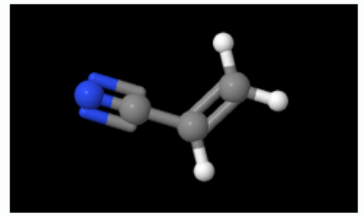
Molecule

ID	185
UID	MOLEC_CH2CHCN
Type	molecule

Names and identifiers

Common name	Acrylonitrile
Secondary names	2-Propenenitrile, prop-2-enenitrile, Cyanoethene, Cyanoethylene, vinylcyanide, Propenitrile, Propenenitrile, CH2CHCN, C3H3N
IUPAC name	2-Propenenitrile
InChI	1S/C3H3N/c1-2-3-4/h2H,1H2
InChI key	NLHHRLWOUZZQLW-UHFFFAOYSA-N
CAS number	107-13-1

Chemical structure and atomic composition



Formula	CH_2CHCN
Chemical formula	CH2CHCN
Stoichiometric formula	C3 H3 N
Structural formula	[CH2]=[CH]C#N
Charge	0
Unpaired electrons	0
Chemical functions number	7
Chemical functions	

Show 10 entries Search:

ID	UID	Type	Number	Common name	IUPAC name	Stoichiometric formula
102	BOND_dCH	bond	3	CH bond	=CH bond	C H
108	BOND_tCCd	bond	1	CC bond	#CC= bond	C2
110	BOND_CdC	bond	1	CC double bond	C=C double bond	C2
138	BOND_CtN	bond	1	CN triple bond	C#N triple bond	C N
407	GROUPMOLEC_RCH2	functional group	1	CH2 group	=CH2 group	C H2
409	GROUPMOLEC_RCHR	functional group	1	CH group	=CH group	C H
420	GROUPMOLEC_RCN	functional group	1	CN group	C#N triple bond group	C N

Showing 1 to 7 of 7 entries

Atoms number 3

Atoms

Show 10 entries Search:

ID	UID	Symbol	Number	Name	IUPAC name	Atomic number Z	Mass number A	Natural mixture
181	ATOM_H	H	3	Hydrogen	Hydrogen	1		Yes
191	ATOM_C	C	3	Carbon	Carbon	6		Yes
195	ATOM_N	N	1	Nitrogen	Nitrogen	7		Yes

Showing 1 to 3 of 3 entries

Natural isotopic composition

Natural mixture Yes

Molecule (2)

Natural isotopic composition
Natural mixture: Yes

Nuclear spin isomer composition
Nuclear spin type: natural

Symmetries
Case: nonlinear-polyatomic

Fundamental vibration modes
Vibrations number: 7
Vibrations

Show 10 entries Search:

Label	Chemical function	Mode	Symmetry	Degeneracy	Fundamental frequency	Observed frequency	Observed frequency 2	Harmonic frequency	Intensity	Activity IR	Activity Raman	Comments
V1	$\geqslant C-H$	stretching		no		3123			s	active		blended with ν_2
V10	$>C=C(-)-C\equiv$	bending		no		788			m	active		
V11	$=C(-)-C\equiv N$	bending		no						active		unknown position
V12	$>C=C<H_2$	wagging		no		971			vs	active		
V13	$>C=C(-H)-C\equiv N$	wagging		no		954			vs	active		
V14	$>C=C<$	torsion		no		682			s	active		
V15	$=C(-)-C\equiv N$	bending		no						active		unknown position
V2	$\geqslant C-H$	stretching		no		3123			s	active		blended with ν_1
V3	$\geqslant C-H$	stretching		no		3042			m	active		
V4	$-C\equiv N$	stretching		no		2240			m	active		

Showing 1 to 10 of 15 entries

Vibrations comments: frequencies of the Q branch, mini between P-R

Properties
Molar mass (g/mol): 53.06
State STP: liquid
Protic: protic
Polarity: polar
Dipole (Debye): 3.92

References and comments
Urls: Wikipedia
NIST Chemistry Webbook
LISA Titan's spectroscopic database
Comments: natural CH_2CHCN

Mineral (1)

Mineral

ID	28
UID	MINER_aragonite
Type	non-silicate mineral

Names

Ima Name	Aragonite
Secondary name	Calcium carbonate

Chemical composition

Formula	$CaCO_3$
Hydration	No
Hydration series	No
Classification level	unique mineral
Chemical formula	CaCO3
Chemical functions number	1
Chemical functions	

Show 10 entries Search:

	ID	UID	Type	Number	Common name	IUPAC name	Chemical formula
	365	IONRAD_CO3	anionic radical	1	Carbonate anion	Carbonate(2-) anion	(CO3)2-

Showing 1 to 1 of 1 entries

Atomic composition

Elemental formula	Ca C O3
Atoms number	3
Atoms	

Show 10 entries Search:

	ID	UID	Symbol	Number	Name	IUPAC name
	191	ATOM_C	C	1	Carbon	Carbon
	198	ATOM_O	O	3	Oxygen	Oxygen
	229	ATOM_Ca	Ca	1	Calcium	Calcium

Showing 1 to 3 of 3 entries

Oxides composition

Oxides

Show 10 entries Search:

Formula	Mass fraction
CaO	56.03
CO2	43.97

Showing 1 to 2 of 2 entries

Mineral (2)

Classification

Strunz class	carbonates - nitrates (05)
Strunz division	carbonates without additional anions, without H2O (05.A)
Strunz family	Alkali-earth (and other M2+) carbonates (05.AB)
Strunz code	05.AB.15
Dana major class	Carbonates, Nitrates, Borates (V)
Dana class	anhydrous carbonates (14)
Dana type	with simple formula A+CO3 (14.01)
Dana group	Aragonite group (Orthorhombic: Pmcn) (14.01.03)
Dana code	14.01.03.01

Crystallography

Crystal system	orthorhombic
Crystal class	dipyramidal
Crystal class symbol	mmm (D2h)
Space group	Pnma

Properties

Molar mass	100.09
Density	2.93

Optical properties

Refringence type	biaxial
Birefringence	0.156
Refringence sign	negatif
Indexes na	1.529
Indexes na ranges	1.529 - 1.53
Indexes nb	1.681
Indexes nb ranges	1.68 - 1.682
Indexes ng	1.685
Indexes ng ranges	1.685-1.686

Optical aspect

Pure color	colorless
True color	colorless, white, grey, yellow
Diaphaneity	transparent to translucent
Luster	vitreous

References and comments

Urls	Wikipedia Webmineral database Mindat Handbook of Mineralogy (Min. Soc. Am)
Comments	Equivalent Space Group: Pmcn (62)

Meteorite - Publication

Object | Matters | Publications | Import history

Object

ID	19
UID	OBJMET_Allende

Type and description

Type	chondritic
Name	Allende
Images	

Show 10 entries Search:

Image	Caption

Showing 1 to 1 of 1 entries

Type

Breccia	false
Type	chondritic
Group	carbonaceous chondrite
Class	CV
Chondrite petrologic type	3
Comments	CVOxA + classified as >3.6 by Bonal et al. (2006)

Global oxides composition

Oxides

Show 10 entries Search:

Formula	Mass fraction
Al2O3	3.27
CaO	2.61
Cr2O3	0.52
FeO	27.15
K2O	0.03
MgO	24.62
MnO	0.18
Na2O	0.45
P2O5	0.23
SiO2	34.23

Showing 1 to 10 of 11 entries

Origin

Reconvery status	fall
Recovery place	village of Pueblito de Allende, Chihuahua, Mexico
Recovery year	1969
Mass	2000000 *g*

References

Urls	Meteoritical Bulletin Database

Publication | Cited publications | Import history

Publication

ID	37
UID	PUBLI_Schmitt_2003
Authors	**B. Schmitt**, S. Rodriguez
Year	**2003**
Title	Possible identification of local deposits of Cl2SO2 on Io from NIMS/Galileo spectra

Type and access

Type	journal
Document type	article
State	published
Access rights	publisher copyright

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 Cl2SO2, with possible contribution by ClSO2, 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 Cl2SO2 and SO2 have been measured to study the selective condensation of these species. Cl2SO2 diluted at ~1% in a millimeter thick layer of solid SO2 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 SO2 ice condensing on plume particles or at Io's surface. The high Cl2SO2 abundance observed implies that a Cl-rich volcanic eruption ([Cl - (Na + K)]/S > 0.015) occurred at Marduk. ClSO2 is a potential additional contributor to the band. Pure H2S is safely discarded as it is extremely unstable at Io's surface but an upper limit of 0.01% is derived for H2S diluted in SO2. Finally, chemical constraints allow us to firmly exclude H2S2. We also suggest that Cl2S 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, Cl2SO2, SO2, H2S, radiative transfer simulation, surface, Io
Contents	instrument-technique, 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

Book

Conference

Links

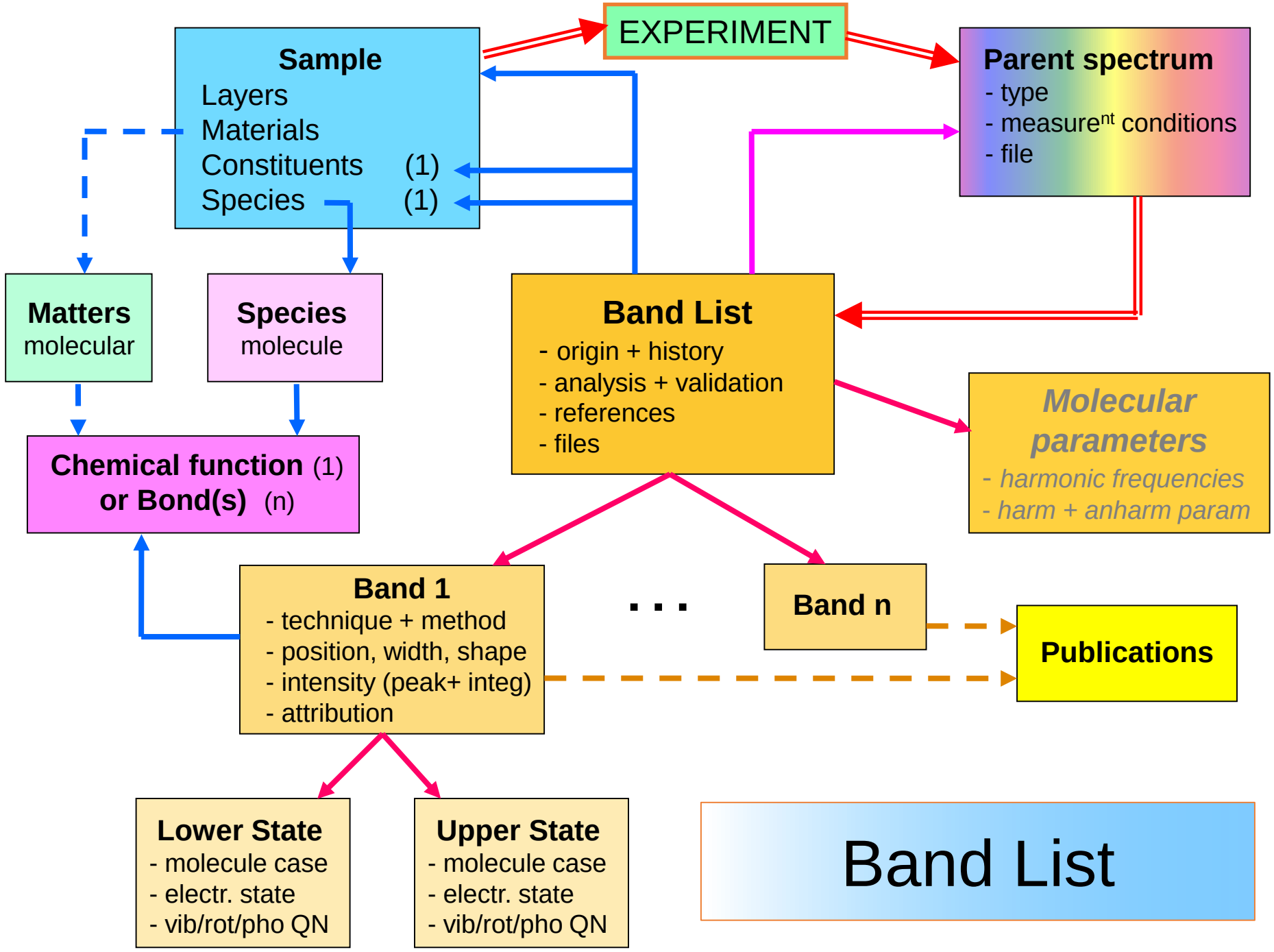
Pdf	schmitt03-JGRE-108-5104.pdf
Doi	10.1029/2002JE001988
Url	http://dx.doi.org/10.1029/2002JE001988
Bibcode	2003JGRE..108.5104S
ADS Url	http://adsabs.harvard.edu/abs/2003JGRE..108.5104S

Fundamental Data feeding: planning

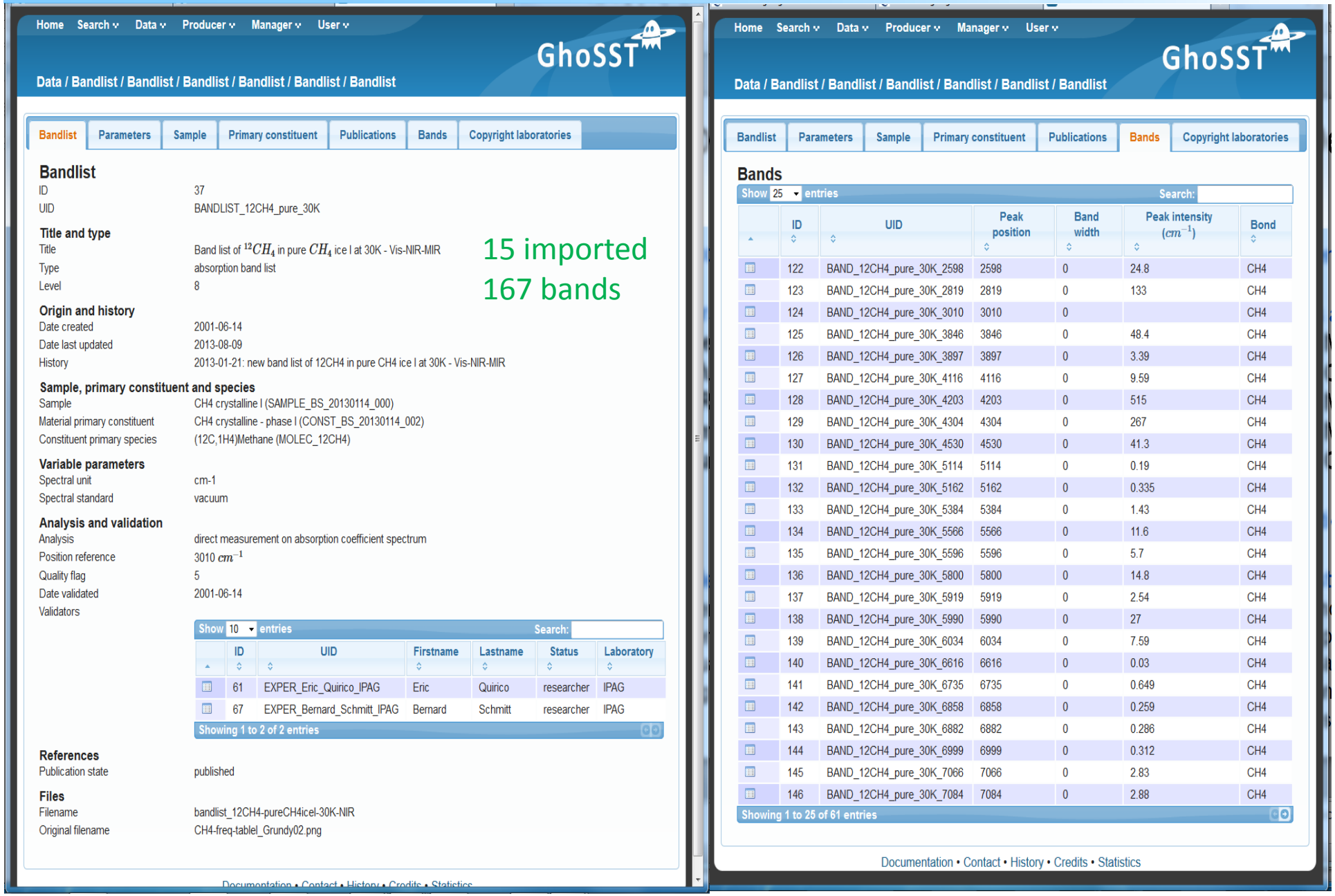
For SSHADE 'Public'	*May 2016*	*Mid 2017*
• Species:		
• Atoms/ Chem Fct	➔ 120 /276	150 /400
• Molecules	➔ 85	130
• Minerals	➔ 104	150
• Matters:		
• Fluid / Minerals / Meteorites	➔ 50	100
• Meteorite objects	➔ 78	100
• Band lists / bands		
• Molecular solids + adsorption	➔ 15 / 167	30 / 250
• Publications	➔ 125	200

Band list : bands and states

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


EXPERIMENT
Sample
Layers
Materials
Constituents (1)
Species (1)
Parent spectrum
- type
- measurent conditions
- file
Matters
molecular
Species
molecule
Band List
- origin + history
- analysis + validation
- references
- files
Molecular parameters
- harmonic frequencies
- harm + anharm param
Chemical function (1)
or Bond(s) (n)
Band 1
- technique + method
- position, width, shape
- intensity (peak+ integ)
- attribution
. . .
Band n
Publications
Lower State
- molecule case
- electr. state
- vib/rot/pho QN
Upper State
- molecule case
- electr. state
- vib/rot/pho QN
Band List

Band list and Bands



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Review the available data for molecular solids

- Partners's data
- Publications

=> critical review and selection

=> selection commitee ?

Tasks of the Scientific Managers and Database Managers

- **Data producers**
  - record spectral data (only part of this EU program if with TNA)
  - analysis of data (idem)

- **Scientific manager**
  - Define which data will by 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

Tasks at IPAG

SSHADE infrastructure development

- Adaptation of SSDM (data model)
- Databases infrastructure
- import tools and validators
- VO interoperability

Coordination of consortium

- Preparation of the common fundamental data of SSHADE
- Development of the common ‘band list database’

Support to partners consortium

- Formation/training of database managers and ‘feeders’
- Preparation of documentations and tutorials for providers

Support to users

- Tutorials & training for users at conferences
- Preparation of documentations and tutorials
- On-line support

Task of the of the SSHADE ‘Support’

SSHADE Database support

- Help to train and support the managers and contributors of the partner databases to prepare and import their spectroscopic data in SSHADE
- 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
- Develop tutorials for SSHADE users. Organize and animate tutorial sessions at various scientific conferences.
- Participate in various types of experiments in different laboratories in order to know well the samples and the various spectroscopic techniques used by the partners.

Task of the of the SSHADE 'Support'

SSHADE database feeding

- Contribute to the preparation and feeding of the fundamental data of SSHADE (molecules, minerals, …).
- Management of some part of these data.
- 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 from data of the SSHADE partners + bibliography.

Scientific activity *(on complementary funds)*

- Improvement, automation and interface of a code for optical constant extraction of ices from transmission spectra. Application to ices from measured spectra.
- Develop methods and numerical codes for optical constant derivation from measurements on powder samples (transmission and reflectance).
- Application to SSHADE data.

http://blog.sshade.eu

The SSHADE blog

http://blog.sshade.eu

- For all general information (partly public / private)
  - Composition of the consortium (+ mailing list)
  - SSHADE Meetings (+ presentations)
  - Reports
  - Presentations at conferences
  - News
  - Links
  - …

The pre-SSHADE database and its documentation

- A new version of **pre-SSHADE database** will be put on-line soon
- Will be the database for:
  - training sessions
  - prepare data files and test data import (before final SSHADE)

A **final SSHADE database** will be made available in 2017

for:

- final import of validated data

Will be put on-line at the delivery of SSHADE database: August 2017

The pre-SSHADE database and its documentation

Contain all necessary documentation

- For data managers (restricted):
  - SSDM data model
  - All xml template files
  - Customized xml files
  - Tutorials for data providers
- For users (public):
  - User manual for SSHADE
  - Tutorials for users
  - Rules for citations

Database implementation by partners

- Training session of managers (2 days)

- Define Who do what in your lab (which partof the work, …)
- Define your feeding plans (which data, …)

- Preparation of basic information and metadata
  - Database
  - Laboratory
  - Experimentalists
  - Instruments
  - Publications

Database implementation by partners

- Preparation of fundamental data
  - Provide list of fundamental data to be used:
    - molecules,
    - Minerals
    - Meteorite
    - Standard matters
  - Contribute to document them

- Preparation of spectral data and metadata
  - Local matters
  - Samples
  - Experiments
  - Spectra

Discussion/questions on database implementation

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