The SSHADE project: a European Database Infrastructure in Solid Spectroscopy

Bernard Schmitt, Damien Albert, Philippe Bollard, Lydie Bonal, Maria Gorbacheva, P. Beck, E. Quirico and the ***SSHADE Consortium Partners****

Institut de Planétologie et Astrophysique de Grenoble, CNRS / UJF

CC BY

Motivations !

- Spectroscopy and spectro-imagery are increasingly used in **space missions**, in orbit or *in situ*, to study small objects of the solar system
- various spectroscopies used to study meteorites and cometary dusts in the laboratory

- large number of laboratories in Europe have developed **experiments to study** the spectroscopic properties of a variety of solid **variety of materials (ices, minerals, organics, …)** of astrophysical interest
- The amount of spectral data collected is huge
- these laboratories boast **leading-edge expertise** in some solid spectroscopy fields.
- However **most of these data**, although published, **are very difficult to access** in a usable form (i.e. electronic) to compare with observation or to use in numerical codes.

➔ We decided to **extend our datamodel** (SSDM) **and our database** (GhoSST) in order to **build a database infrastructure able to distribute the spectroscopic data** of most of the European laboratories

What is *SSHADE ?*

"Solid Spectroscopy Hosting Architecture of Databases and Expertise"

It is an **European project** of a **set of databases (~20)**

to provide the community with spectra

of solids (***ices***, ***minerals***, ***organics***, ***cosmo-materials***, ***…***)

of astrophysical and terrestrial interests

in the **X-ray to sub-mm range**.

Consortium: SSHADE Partners

- 20 groups in 18 laboratories
- 8 countries: F, GB, E, I, CH, D, PL, HU
- Expertises in:
  - Solid materials:
    - ices, minerals
    - organics, inorganics
    - meteorites, IDPs, ...
    - optical materials, ...
  - Various spectroscopies:
    - transmission, reflection,
    - photometry, Raman, XANES ...
  - Various spectral ranges
    - X, UV, Vis, NIR-FIR, sub-mm

The SSHADE Partners: 20 (8 countries)

- **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, Cristian 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, M. Angel Moreno)
- **LATMOS / IMPEC**, Institut Pierre Simon Laplace - F (Nathalie Carrasco)
- **LGL-TPE / ENS-Lyon** - F (Bruno Reynard, Gilles Montagnac (exp.), Razvan Caracas (th.))
- **Konkoly Astronomical Institute** – HU (Akos Kereszturi)
- **Planetary Geology Laboratory**, PAS – PL (Joanna Gurgurewicz, Luigi Castaldo)
- **Clay Minerals Laboratory**, PAS– PL (Arkadiusz Derkowski, Luigi Castaldo)
- **ESRF / FAME line**, Grenoble – EU / F (Denis Testemale, Isabelle Kieffer)

Data of SSHADE

- **Spectral ranges**:
  - from X to sub-mm

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

- **Data types**:

➢ **Spectra**
- infrared transmission spectra, absorption coefficients, optical constants
- Raman spectra et micro-spectroscopy
- reflectance spectra of surfaces, spectro-photometric functions
- multispectrale 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 (spectral and composition maps**)** of natural et synthetic 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**
  - multispectral and multi-angular imagery of mineral surfaces
  - multispectral photometric fonctions
  - FIR+sub-mm spectra and absorption coefficients of synthetic silicates
- **LISA**
  - MIR spectra of ices and organic polymers
- **LATMOS**
  - MIR spectra of synthetic organics (tholins, ...)

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.
- **LGL-TPE, ENS-Lyon**
  - Experimental and theoretical Raman spectra of minerals and meteorites
- **Open University**
  - VUV spectra of ices
- **IAPS**
  - Spectra of meteorites, minerals and rocks
- **Univ. of Bern**
  - multi-bands bidirectional photometry of various materials: ices, organics, mixtures, ...
- **AIU Observatory** [DOCCD 'database']
  - optical constants 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
- **Planetary Geology Laboratory**
  - NIR spectra of basalts and organics
- **Clay Minerals Laboratory**
  - NIR+MIR spectra of well characterized clay minerals

What is *SSHADE ?*

"Solid Spectroscopy Hosting Architecture of Databases and Expertise"

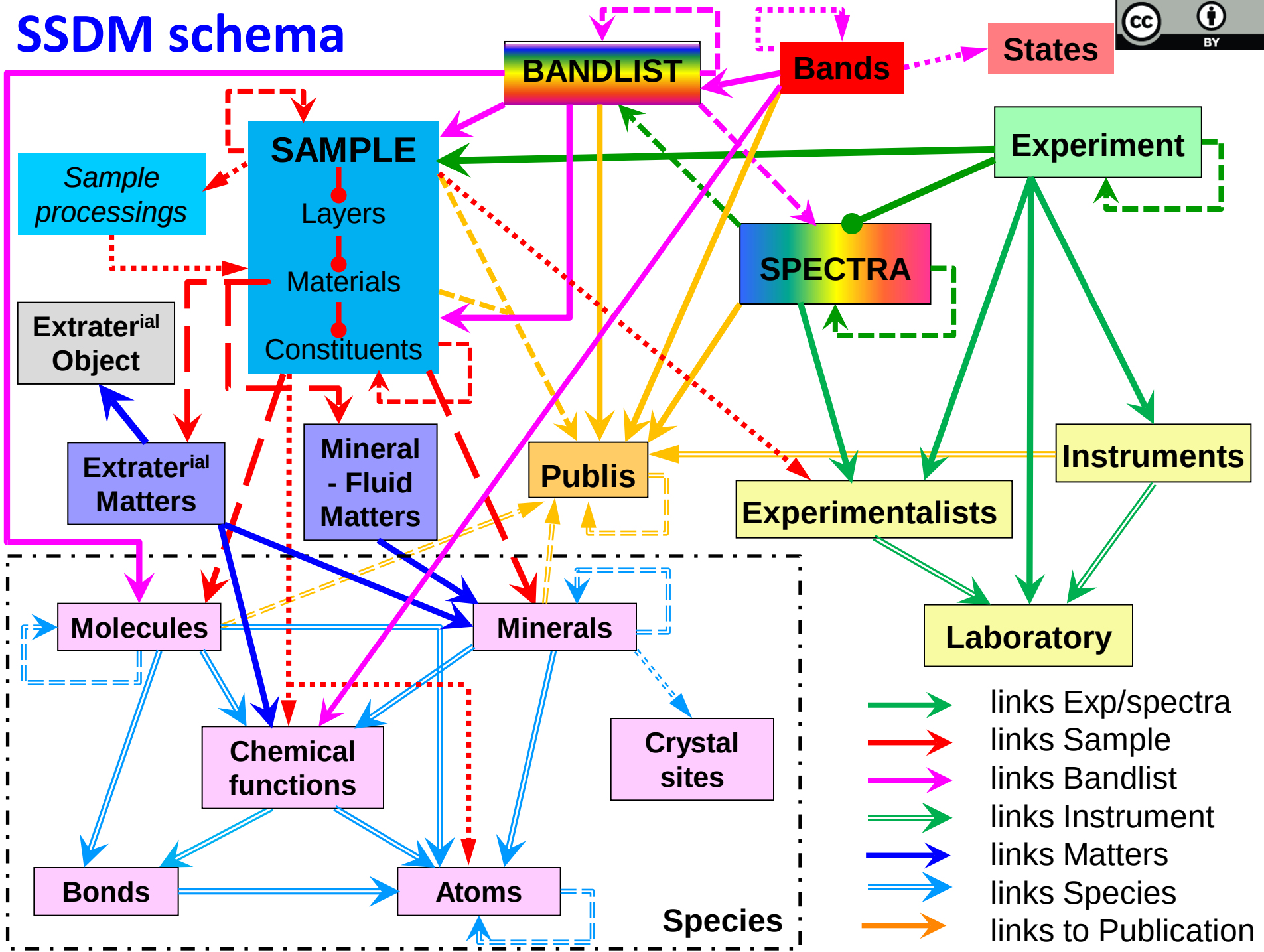
It is a set of databases (~20) **based on**

the Solid Spectroscopy Data Model (SSDM)

and **building on the GhoSST database interface**

Gho SS DM T HADE

SSDM schema


BANDLIST
Bands
States
SAMPLE
Layers
Materials
Constituents
Sample processings
Experiment
SPECTRA
Extraterial Object
Extraterial Matters
Mineral - Fluid Matters
Publis
Instruments
Experimentalists
Laboratory
Molecules
Minerals
Chemical functions
Crystal sites
Bonds
Atoms
Species
links Exp/spectra
links Sample
links Bandlist
links Instrument
links Matters
links Species
links to Publication

Search(s) Spectra + Bandlists

CC BY

View results | 6 spectra found

Material

Species type: -- All --, ***Molecules***, Molecule, Molecular ion

Species formula: H2O — Species symbol, stoichiometric formula or structural formula

Species name and code:

Species relevance: -- All --, ***Molecules***, Actual, Precursor

Matter origin: -- All --, Terrestrial, Extraterrestrial, Synthetic

Material name:

Matter family: -- All --, Molecular, Mineral, Rock

Temperature min. (K): 15

Temperature max. (K): 300

Layers number:

Layer texture: -- All --, Loose granular, Cemented granular, Sintered granular

Constituents mixing: -- All --, Single phase, Multi-phases, Coated grain

Constituent family: -- All --, Molecular solid, Molecular liquid, Molecular gas

Phase type: -- All --, Crystalline, Amorphous, Glassy

Species compound: -- All --, Pure, Mixed, Binary

Ad/absorption: -- All --, Adsorption, Insertion, No

Instrument

Type: -- All --, FTIR spectrometer, Grating spectrometer, AOTF spectrometer

Technique: -- All --, Transmission, Reflection, Biconical reflection

Spectral range

Unit: cm-1

Type: ----- All -----, FIR, MIR, NIR

Custom min.:

Custom max.:

Spectrum

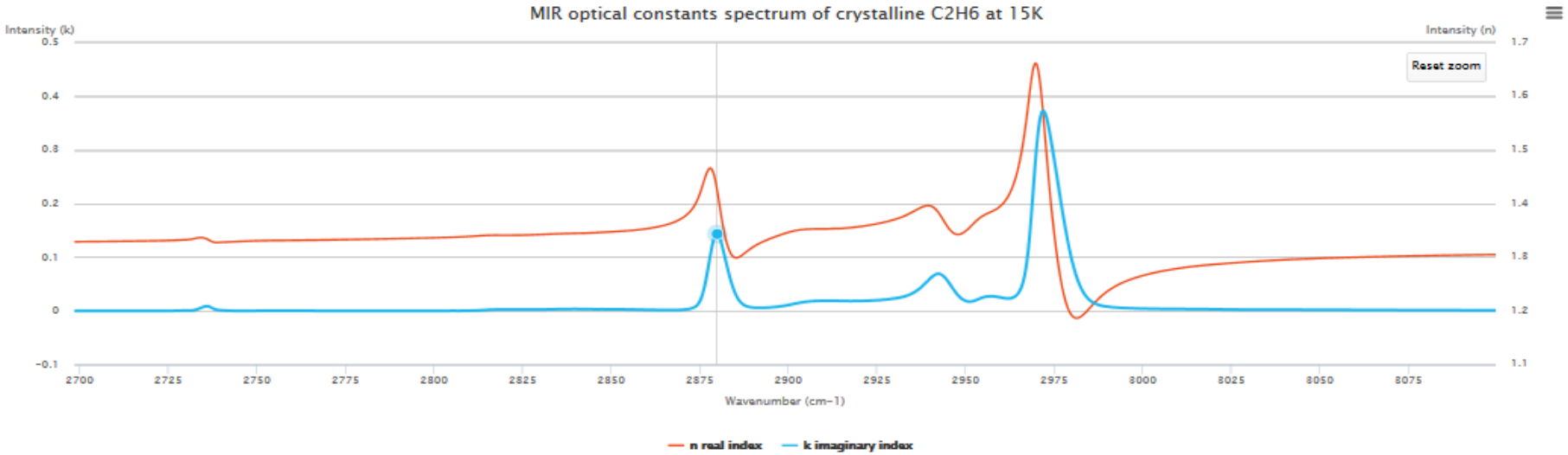
Type: -- All --, Bidirectional reflectance

View Spectra + Metadata

GhoSST

Graph

Export this spectrum | Compare this spectrum



Point details

Wavenumber (cm-1)	2879.886
k imaginary index	0.1436379

Settings

Display	Errors: Infos:
Unit	cm-1
Scale	X: Linear Y left: Linear Y right: Linear
Colors	K: 1CB5ED N: EB4513
Zoom	Full range Valid range

Spectrum

ID	474
UID	SPECTRUM_BS_20130205_003
Spectrum type	optical constants
Title	MIR optical constants spectrum of crystalline C2H6 at 15K
Valid range	670.00-3660.00 cm^{-1}
Created	1996-01-01
Last updated	2014-08-15
Analysis	Iterative inversion of n and k with full optical model of the film+substrate + Kramers-Kronig analysis over 670-3660cm-1 range and n(15800cm-1, CH4)= 1.36 (F. Trotta thesis 1996) - k is set to 0 and n is smoothed outside C2H6 bands to reduce noise and the CO2 impurity band (2357.5 cm-1) is removed by interpolation
Quality flag	4

More details...

Sample

ID	305
UID	SAMPLE_BS_20130205_003
Name	C2H6 crystalline - dep 15K
Number of layers	1

CC BY

Export Spectra + Metadata

CC BY

Spectra

Actions	ID	Type	File title	Spectral range min	Spectral range min	Sample temperature	Species	Date
View ☐	10	transmission	N87_S09 CH4 ICE 30 K	1850	10500	-	-	2011-08-04
View ☑	94	bidirectional reflectance	NIR-MIR bidirectional reflection spectrum (i=0°, e=30°) of Smectite SWy-2 with adsorbed H2O at -30°C an P(H2O)= 0.25 mbar	1.2	2	-	-	2011-10-01

Wavenumber/Wavelength/Frequency

Unit	µm
Format	Float
Number of significant digits	10
Number of decimals	3

Value/Intensity

Format	Scientific (e)
Number of significant digits	11
Number of decimals	5

Spectra data file

Type	Spectrum data with short header
Format	ASCII

Export archive file

Filename	snow-NIR
Compression type	.zip (Zip)

Download

Hosting Solid Spectroscopy data of European Data Providers: *SSHADE*

- 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
  - ✓ A common bandlist database

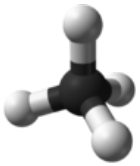
- Also direct link from each individual DB web page (powered by SSHADE)

- All databases/engines hosted at OSUG data center (OSU Grenoble - UJF)

- SSHADE will be a service of others VO (VESPA (*Europlanet-VO*), VAMDC, ...)

GhoSST: SSDM General Structure

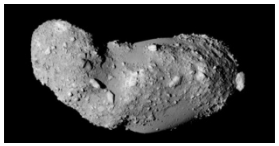
CC BY

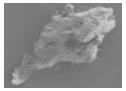


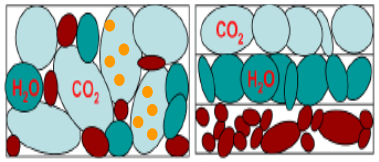
SPECIES

MATTERS

OBJECTS

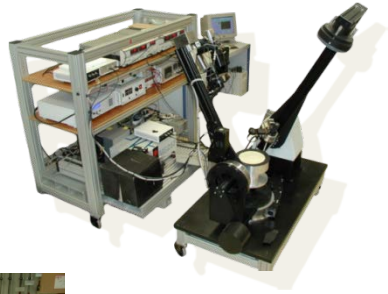


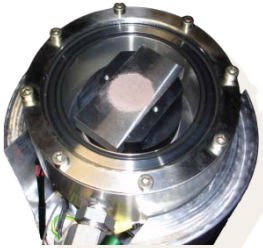




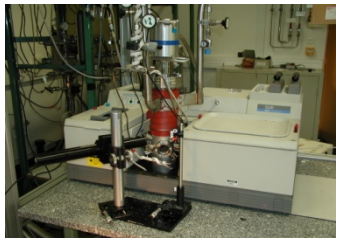
SAMPLE

INSTRUMENT



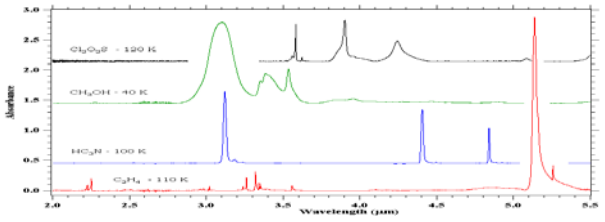


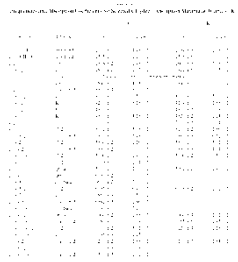
EXPERIMENT



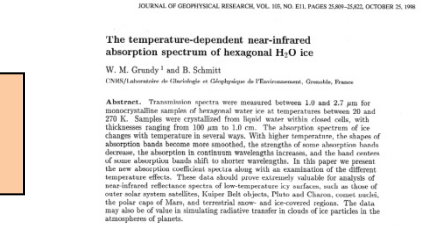
BAND LIST

SPECTRA





PUBLICATIONS



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

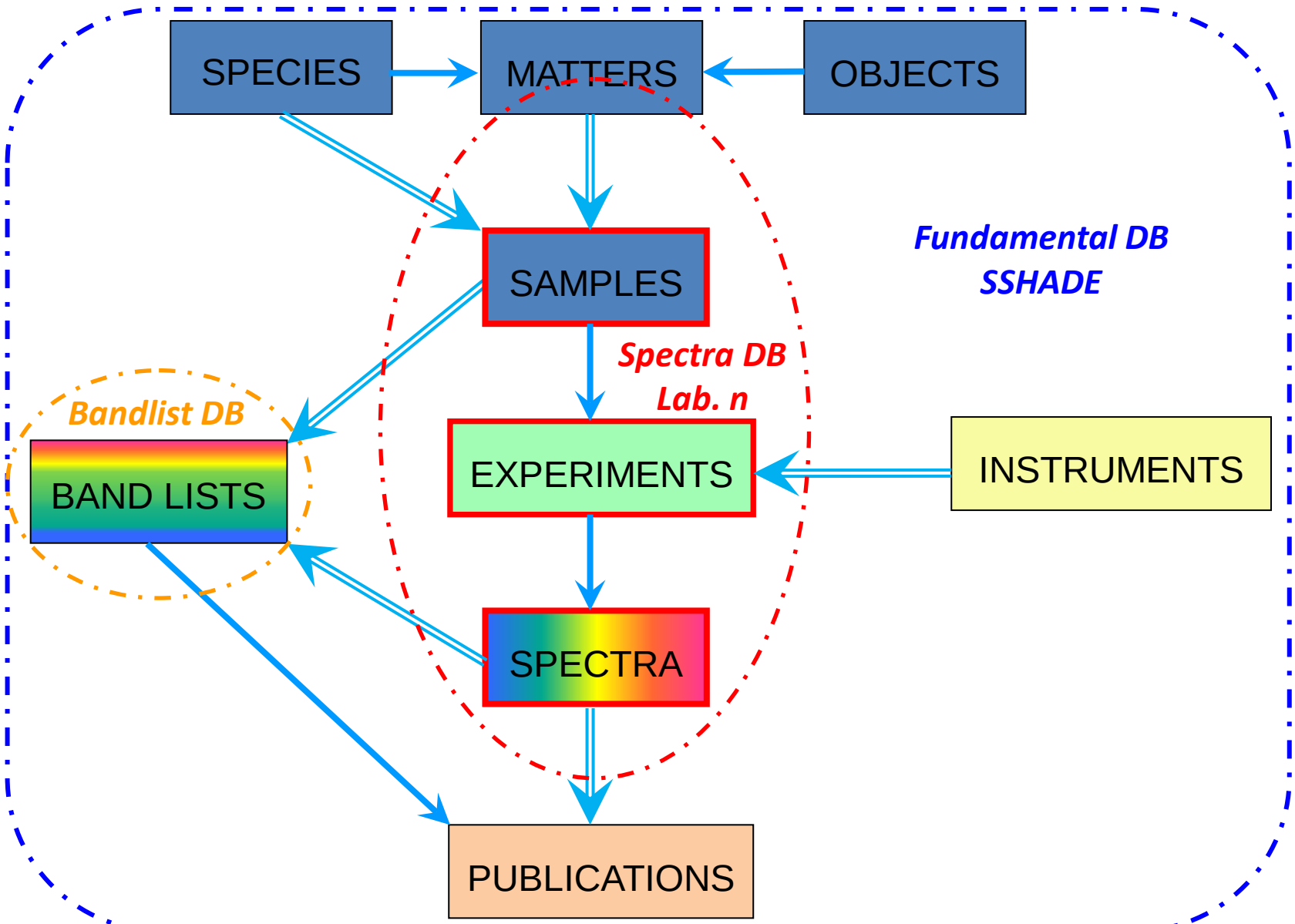
The temperature-dependent near-infrared absorption spectrum of hexagonal H_2O ice

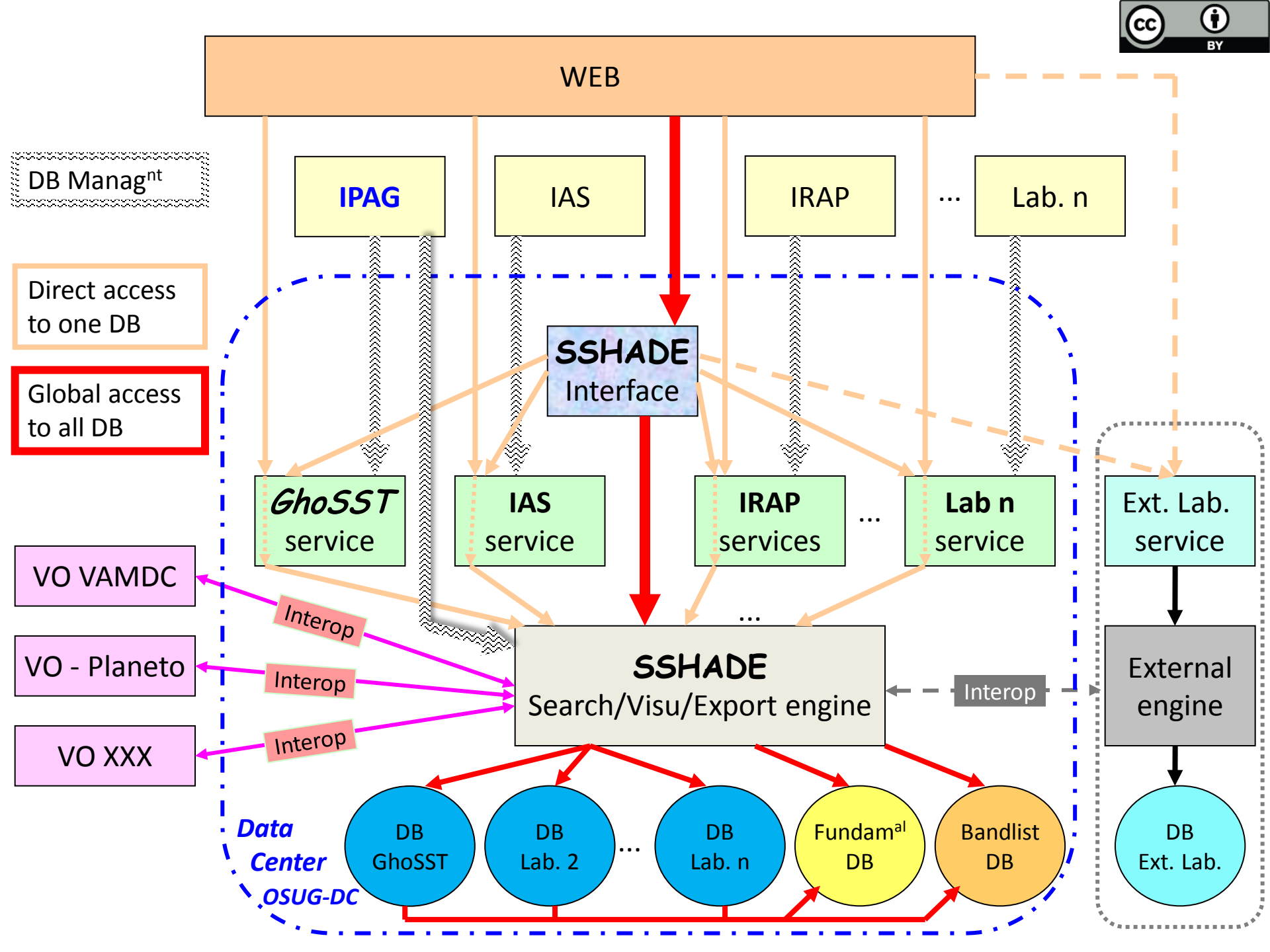
W. M. Grundy[1] and B. Schmitt

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




WEB
DB Managnt
IPAG
IAS
IRAP
...
Lab. n
Direct access to one DB
Global access to all DB
SSHADE Interface
GhoSST service
IAS service
IRAP services
...
Lab n service
Ext. Lab. service
VO VAMDC
VO - Planeto
VO XXX
Interop
Interop
Interop
...
SSHADE Search/Visu/Export engine
Interop
External engine
Data Center OSUG-DC
DB GhoSST
DB Lab. 2
...
DB Lab. n
Fundamal DB
Bandlist DB
DB Ext. Lab.

CC BY

SSHADE Project

- **Done:**
  - Feb. 2014 : **first SSHADE-Europe meeting**
  - mid-2014: start 2-3 new DataBases (in pre-SSHADE structure)
  - sept. 2014 Europlanet-RI proposal (*Horizon 2020):* VESPA WPs

- **Project:**
  - mid-2015/17: **develop SSHADE infrastructure**
    (if Horizon 2020 funding)
  - 2015/19 prepare data for ingestion (in pre-SSHADE structure)
  - 2017: ingest all data in SSHADE database
  - 2017: **open first SSHADE DataBases (~6-8) to 'users'**
  - 2019: **≥ 18 databases open to 'users'**

to follow SSHADE: **http://blog.sshade.eu/**