SSHADE in H2020: Development of an European Database Infrastructure in Solid Spectroscopy

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Introduction

Spectroscopy and spectro-imagery are increasingly used in space missions, in orbit or in situ, to study the solid phase of the objects of the solar system (e.g. VIMS/Cassini, DISR/Huygens, VIRTIS/Rosetta, RALPH/New Horizons, …): icy, mineral or organic surfaces and grains, dust particles, aerosols, etc. **Infrared, Raman, fluorescence and X-rays micro-spectroscopies** are used to study meteorites and cometary dusts in the laboratory and onboard some space missions for in situ measurements. A major contribution to the analysis of these observations is the **measurement in the laboratory of UV, Visible, IR, Raman and XANES spectra of a variety of materials** (ices, minerals, organics, …) expected to be present at the surface of THE bodies of the solar system or in their ejected grains (e.g. comets, asteroids, TNO, icy satellites, Pluto, Mars, …).

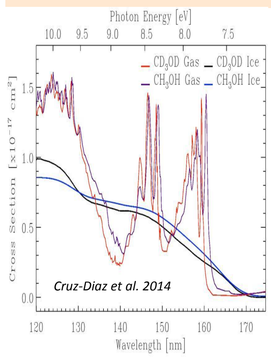
Solid spectroscopy data in Europe

A large number of laboratories in Europe have developed experiments to measure and study the spectroscopic properties of a variety of solid materials of astrophysical interest, either natural (terrestrial or extra-terrestrial) or synthetics. **The amount of data collected is huge** and several of these **laboratories boast leading-edge expertise in some solid spectroscopy fields**. However most of these data, although published, are very difficult to access in an usable form (i.e. electronic) to compare with observation or to use in radiative transfer codes.

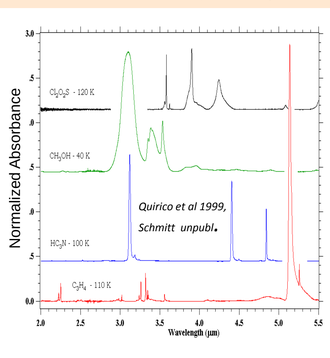
We thus decided to extend our datamodel (SSDM) and expand the GHOSST database structure (http://ghosst.osug.fr) to **build a database infrastructure able to gather and distribute the spectroscopic data of most of the European laboratories** working on solids of any type with astrophysical and terrestrial applications

Solid planetary materials in SSHADE

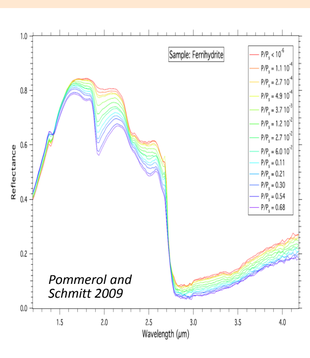
- Ices, hydrates, clathrates, … + irradiation
- Organic solids: simple, macromolecular materials, polymers, …
- Rocks, minerals, salts, hydrated materials, adsorption, …
- Other compounds (sulphur compounds, …) + irradiation
- Natural and extra-terrestrial samples (meteorites, IDP's, Stardust, …)



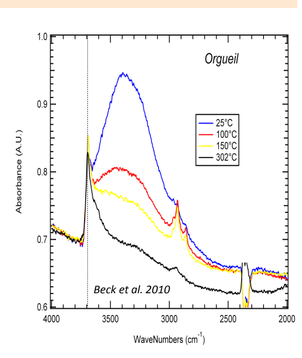
Ices (UV)



Organic solids (MIR)



Hydrated minerals (NIR)



Meteorites (MIR)

What is SSHADE?

SSHADE ("Solid Spectroscopy Hosting Architecture of Databases and Expertise") is a **project of a set of databases on solid spectroscopy** that is starting its development in September 2015.

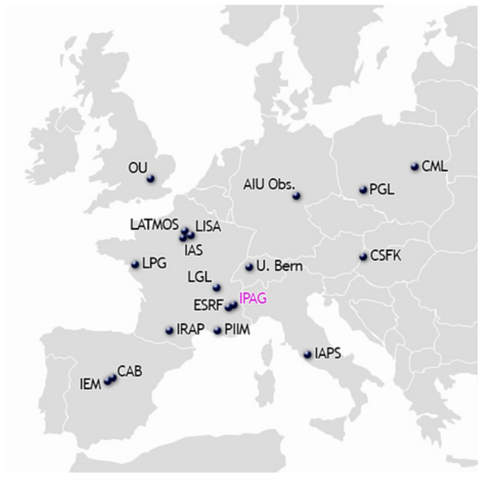
The **SSHADE databases** will cover laboratory, field, airborne as well as simulated and theoretical spectral data with their corresponding spectra and their **various types of products** (ex: transmission, absorbance, absorption coefficient, optical constants, band list) **for many different types of solids**: ices, snows and molecular solids, minerals, rocks, inorganic solids, natural and synthetics organic and carbonaceous matters, meteorites and other cosmomaterials, … **with a wide range of measurement technics**: transmission, bidirectional reflection, Raman, fluorescence, … and **over a wide range of wavelengths**: from X-rays to millimeter wavelengths (can be extended up/down).

It is **based on the GhoSST database developments** (Europlanet-RI + VAMDC 2009-2012). The SSHADE database infrastructure will be hosted at the OSUG Data Center (University of Grenoble Alpes). The SSHADE project was initially boosted by INSU/CNRS who asked us to develop a "thematic pole on planetary solids" within the new framework of observation services of INSU. The SSHADE development is **part of the VESPA activity within the European e-infrastructure Europlanet 2020-RI** of the Horizon 2020 program (09/2015-08/2019).

The SSHADE-Europe Consortium

The SSHADE consortium has currently **20 partner groups** in **18 laboratories** from **8 different European countries** (F, UK, I, D, E, HU, PL, CH). News about this project can be followed on the SSHADE blog: http://blog.sshade.eu

- **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)

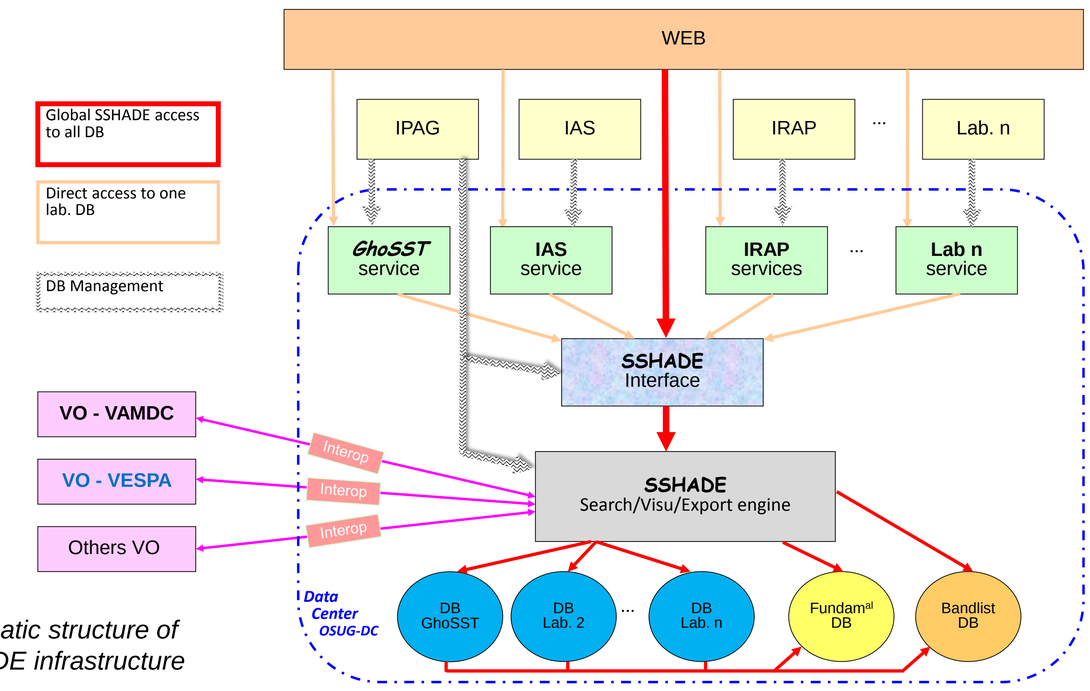


SSHADE infrastructure

The SSHADE infrastructure will have:
- A common 'solid spectroscopy' interface
- A common Import / Search / Visualization / Export engine
- A common fundamental database (species, publications, objects, band list, …)
- A set of spectral databases: one per group/laboratory (GhoSST is one of them)

It will be possible either to **search all databases at the same time** with various filters (spectrum type, species or material type or name, …), and from different points of view (spectra, band lists, publications, objects, …), or to select the target database(s).

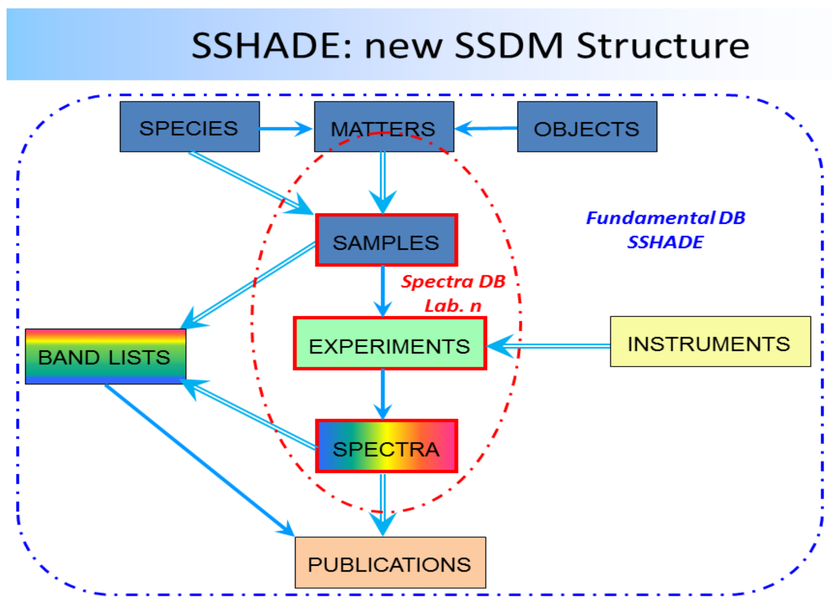
SSHADE will be also a service for Virtual Observatories (VESPA, VAMDC, ...).



Schematic structure of SSHADE infrastructure

SSDM evolutions for SSHADE

The **transformation of the GhoSST database structure into the SSHADE infrastructure** will need a number of modifications such as the separation of the fundamental databases (species, publications, objects, …) from the individual spectroscopic databases (one per laboratory) and the rewriting of the data queries (mono to multi DB). Each database will be also customized to its effective content (types of solids, of spectra, …) for easier search. This work will be mostly devoted to IPAG.



Schematic structure of SSDM for the SSHADE infrastructure

SSHADE Databases implementation

The databases of each of the 20 partners of the SSHADE consortium will be progressively implemented in the SSHADE infrastructure all along the 4 years of the program. Each of the groups have a **Scientific manager** (responsible of the scientific content of the database and it quality) and a **database manager** (responsible of the ingestion of the data in the database), as well as **contributors** (experimentalists who produce data) to develop the content of their database. They will also contribute to the **common 'band list' database of molecular solids** by providing band parameters data or critical reviews of published data.
They will be trained to the tools developed for data preparation, validation, ingestion and management. Tutorials for the database users will be also organized mostly during major planetary sciences and astrophysics conferences. The **SSHADE web site** will contain all documentation on the SSDM data model, the use of the SSHADE database, tutorials, as well on the experimental systems and cells used to record the spectra.

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