

# Virtual Atomic and Molecular Data Centre

<http://www.vamdc.eu> (.org)

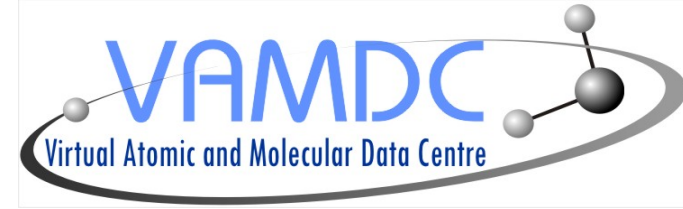
## Introduction and Highlights

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# VAMDC Current Status



## Initial Consortium

- **21 Partners**= 15 EU Universities, 4 Russian and 1 Venezuelan Institutes
- **3 External partners in USA:** Harvard University (HITRAN), JPL Spectroscopy Database/NASA, NIST Atomic Linelists
- **1 Associated partner** : IAEA Atomic Data Division

## Initial Databases and Technological Centers

20 Databases developed and maintained at partner institutes

- 7 Atomic DB
- 11 Molecular DB
- 2 Solid Spectroscopy DB
- Different processes: Linelists, collisions, reactions, ...

Initial State: **Heterogeneous** queries and output formats

4 Technological Centers:

- **VO-Paris**, Paris Obsv., France: P. Le Sidaner, M.L. Dubernet
- **Cambridge, IoA, UK**: G. Rixon, N. Walton
- **Uppsalla, Sweden**: N. Piskunov
- **UCL/MSSL, UK**: J. Tennyson, K. Benson

➔ **now interconnected**

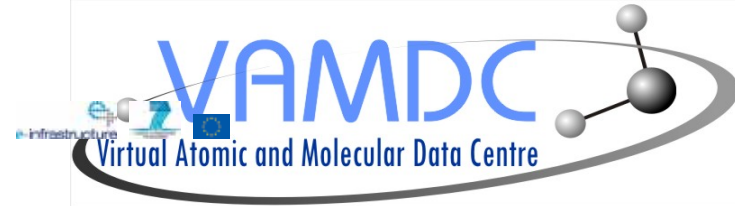
# VAMDC Highlights



- 2 Releases of standards in P3, last in July 2012
- Last Release of Infrastructure = Level 3 in June 2012
  - Software such as Node Software, Tools such as TAPVALidator, SPECTCOL
  - Portal in its current Robust form
  - Consumer services
  - Species Database
  - Taverna Plugins
  - Implementation at VAMDC Nodes
- See Day 1 Talks and Poster Session

# VAMDC Highlights

- 2 Regional Meetings in Russia and Serbia in 2012 and 1 south america meeting planned in January 2013.  
→ See Presentations on Friday by V. Perevalov, M. Dimitrijevic, C. mendoza
- A VAMDC-USA meeting in October 2012  
→ See feedback : Talk of Y. Ralchenko (Thursday)
- A 2 years EU support (small project) via SUP@VAMDC → « SUP » meaning « SUPPORT »



### SUP@VAMDC SUMMARY

Atomic and molecular (A+M) data are critical for a range of applications such as astrophysics, atmospheric physics, fusion, environmental sciences, combustion chemistry, health and clinical science including radiotherapy. They underpin industries ranging from technological plasmas to lighting. The Virtual Atomic and Molecular Data Centre (VAMDC) is a major new European initiative that has built a unified, secure, documented, flexible and interoperable e-science environment-based interface to 24 existing A+M databases.

SUP@VAMDC will coordinate collaborative studies and provide the supporting procedures that will develop a global e-infrastructure for the assembly, curation and access to A+M data. It will adopt and adapt VAMDC protocols to include further A+M databases and networks around the world. It will also design the pathways by which common policies may be developed for an open science version of VAMDC that will extend its availability to new audiences such as schools, students, citizens and industry.

### SUP@VAMDC ACTIONS

- Provide operational, legal and technological support for studies aimed at developing a sustainable open scientific data e-infrastructure in Atomic and Molecular Data.
- Provide support and the medium for inclusion of authentication, authorization and accounting as well as licensing and tools within the VAMDC brand.
- Promote and fashion future interoperability (technical, semantic, reference architecture, etc) across the A+M community through promotion, monitoring and adoption of common standards.
- Implement a programme of dissemination to raise the visibility of the VAMDC e-infrastructure to new audiences such as other disciplines, which could use the VAMDC e-infrastructure in their own scientific endeavours as well as students and citizen-scientists.

- Develop a globally connected and interoperable VAMDC e-infrastructures between the EU and the rest of the world, including Brazil, South Africa, Asia, Australia, USA, through hosting workshops and supporting dialogue between synergistic structures.
- Analyze and evaluate possible business models for supporting an open science model (OPEN VAMDC) while assessing which model(s) can provide financial sustainability for VAMDC itself.

### SUP@VAMDC OUTPUTS

- A worldwide open science e-infrastructure based on an international consortium of atomic and molecular databases providers linked by international agreements and common policies by which A+M data providers present and curate their data.
- A worldwide e-infrastructure impacting A+M Users: Astrochemistry and Planetary Sciences, Atmospheric Science, Fusion Energy Research, Lighting and Plasmas technologies, Radiation Sciences.
- A worldwide e-infrastructure with a wide public outreach impacting industrial and commercial partners, citizen science and education.
- Develop a roadmap to establish an accessible worldwide Open Science e-infrastructure constructed and operated by an international consortium of A+M database and service providers.

### AT A GLANCE

**Project Title :**  
Support at the Virtual Atomic and Molecular Data Centre

**Duration :**  
December 2012-November 2014

**EC Funding :**  
750 000 Euros

**Programme :**  
FP7 INFRASTRUCTURES-2012-1;  
INFRA-2012-3.3

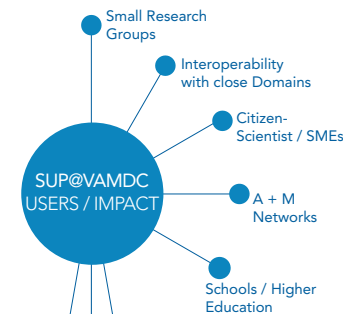
**Project identifier :**  
313284

### Partners :

- Observatoire de Paris, France – Coordinator
- The University of Cambridge, UK
- Uppsala Universitet, Sweden
- Open University, UK
- Universitaet zu Koeln, Germany
- University College London, UK
- Korea Atomic Energy Research Institute, South Korea
- University of South Africa, South Africa
- Tata Institute of Fundamental Research, India

### EXTERNAL AND ASSOCIATED PARTNERS :

- Yuri Ralchenko, Atomic Spectroscopy Group, NIST, USA
- Laurence S. Rothman, The Harvard-Smithsonian Center for Astrophysics, Cambridge, USA
- Brian Drouin, JPL, California Institute of Technology, USA
- Carlos Gonzales, The Chemical and Biochemical Reference Data Division, NIST, USA
- Milton M. Fujimoto, Departamento de Física, Universidade Federal do Paraná, Brazil
- Stephen Buckman, Atomic and Molecular Physics Laboratory, Australian National University, Australia
- Michael Brunger, The Electron Scattering and Modelling Group, Flinders University, Australia
- Izumi Murakami, National Institute for Fusion Science, Japan
- Bas Braams, Atomic and Molecular Data Unit, IAEA, Austria

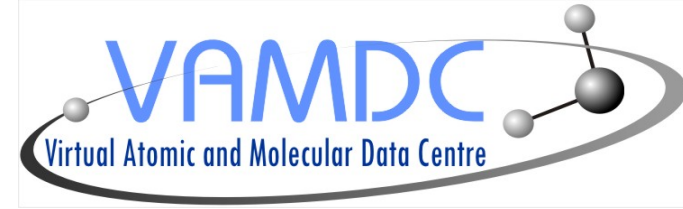


### WORLD CONNECTED

**Coordinator :**  
M.L. Dubernet, Observatoire de Paris,  
marie-lise.dubernet@obspm.fr  
Links :  
Project SUP@VAMDC website : [sup-vamdc.vamdc.eu](http://sup-vamdc.vamdc.eu)  
VAMDC website : [www.vamdc.eu](http://www.vamdc.eu) or [www.vamdc.org](http://www.vamdc.org)  
Access to Databases : <http://portal.vamdc.eu>

# SUP@VAMDC

(2 years starting Dec. 2012)



- Extension through EU support to India, South Africa, Brazil, USA, South Korea, Japan, Australia
  - First meeting in the USA – October 2012 at ICAMDATA, NIST -
- Link to evaluation groups: APAN, DCN (IAEA)
- Support to new databases
- Support to use our libraries in user's software
- Outreach towards schools, high education, SMEs, citizen-scientist
- Build an International Consortium with Status

# VAMDC Current Scope

- Exchange of data and information on Gas Phase Processes/Description of States
  - >> Through XSAMS Schema (currently VAMDC XSAMS version 1.0)
  - >> Full interoperability
- With Solid Spectroscopy
  - >> Interoperability through key words for some data
  - >> Tools should become available and distributed to handle solid spectroscopy data and have real working use cases

# VAMDC/SUP@VAMDC Issues



- Could we extend to more databases/close fields (Thursday) ?
  - Some with little changes ? (J. Postler, L. Pitchford, Y. Ralchenko)
  - Some by extending the XSAMS schema ? How to interact with domains that are close ?
    - Invited Guests in **Panel 1**: P. Garrigues « Chemistry for the environment » (ISM Lab. Director and SAB Member, Bordeaux), S. Mazevet « Condensed Phase » (LUTH Director, Obs Paris)
  - **Tech 1** session on Thursday's afternoon



# VAMDC/SUP@VAMDC Issues



- Are we ready to meet user needs (Wed. & Friday) ?
  - Atmospheric Applications (J. Orphal, IMK, Germany)
  - Interstellar Medium (C. Vastel)
  - Planetology (S. Erard)
  - **Tech 2** session on Friday for implementation of libraries, spec. Of tools for user applications
  - **Panel 3** (Friday)
- Future Technological Issues
  - Talk of A. Fazliev (Friday), See poster of Dr Kovacevic
  - **Tech 1** (Thursday Afternoon)
  - **Panel 3** (Friday)

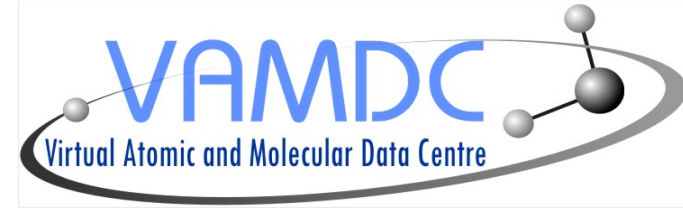
# VAMDC/SUP@VAMDC Issues



- Impact of VAMDC with references – Open VAMDC
  - Talk by M. Ohishi on World data System (Thursday)
  - IoPP View by Mrs I. Auffret-Babak, IoPP representative
  - **Panel 2** Discussion
- Outreach towards school, high education, SME
  - Talk of AL Melchior on « Hands on Universe »
  - **Panel 3** combined with Future lines (Friday)
- Connection to Data Evaluation Groups
  - Talk by Bas Braams about IAEA work
  - Views from VAMDC members
  - **Panel 4**

# VAMDC/SUP@VAMDC

## Issues: Political Roadmap (Board)



- Create an association under Belgium law
  - Linked to a VAMDC charter describing different issues such as quality charter, duties and rights, etc...
- Decide at board to create such association and get a « real committee » from different countries to write status
  - General Assembly with members
  - Exec Committee elected by the G.A.
    - Propose strategy to G.A.
    - Negotiated how association can be supported by different projects of members, etc...
    - Propose names of scientific/technical responsibilities → operational

# Operation of VAMDC Consortium After 2012: no pyramidal organisation



- « **Infrastructure Team** » : to make sure that current infrastructure is working
  - To be contacted for support to existing infrastructure
  - Proposed Names of people in charge (PC) : G. Rixon, P. Le Sidaner
- « **Innovation Team** » : to upgrade Standards taking into account new data
  - To be contacted if you want to join, and you don't know whether your data can be described in the current infrastructure
  - Proposed Names (PC): F. Delahaye, C. Hill
- « **Software Team** » : to upgrade softwares, develop new applications, assess external softwares
  - Proposed Names (PC): new Senior Engineer, N. Moreau
- « **Training Team** » : about the existing infrastructure
  - Organize Tutorials (initiated by VAMDC or on demand)
  - Individual trainers sent to Nodes and to Users (on demand)
  - Proposed Names (PC): New Senior Engineer, + ?
- « **Outreach/Media team** »
  - Proposed Names (PC): ??
- « **Science team** »
  - Connection to Evaluation group
  - Connection to User needs
  - Proposed Names (PC): ??

# What can be expected from this meeting ?



- From Panels discussions: Some useful lines of work and ideas
- From Tech 1 and Tech 2 sessions: A program of work for next year (and long term issues)
- From Board: Approval of association and designation of a group for writing the status (not always the same)
- From All+ Board: Names of people willing to take responsibilities of Teams and actively participate
- Friday's afternoon: we should give feedbacks on all the above points