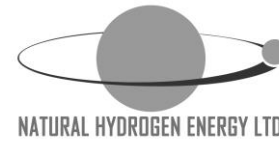
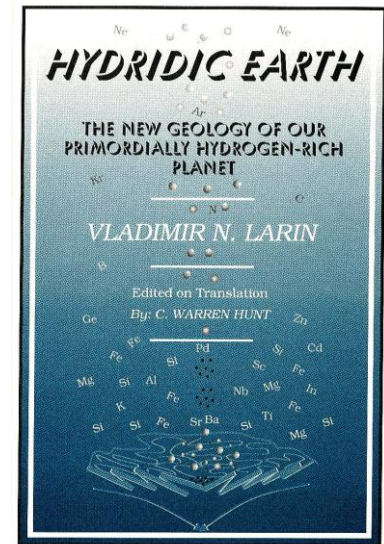
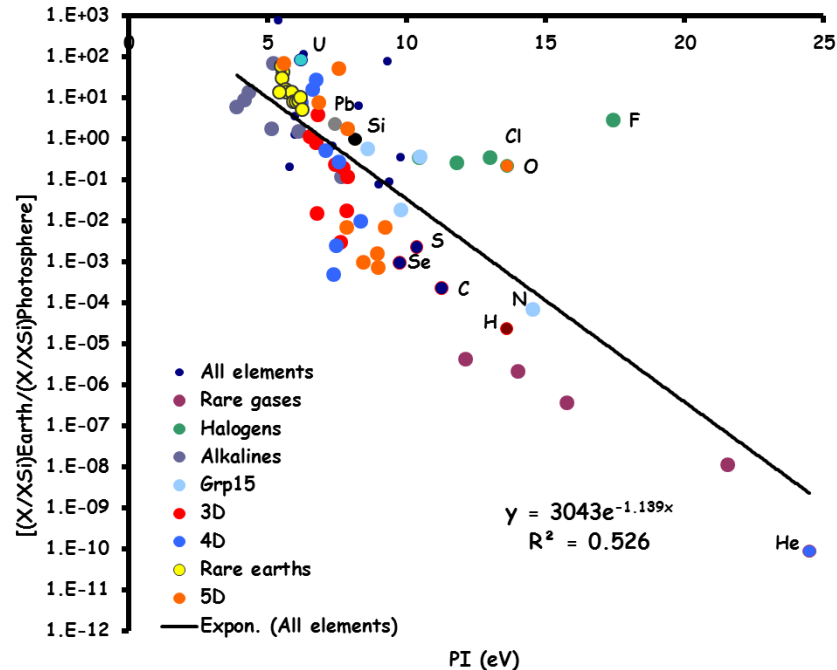


# Primordially hydridic Earth

Viacheslav Zgonnik, Hervé Toulhoat, Vladimir Larin, Nikolay Larin



Abundances of elements on Earth's crust relative to Sun's photosphere and Si plotted versus first ionization potential (IP)



- Clearly shows separation of elements by their IP
- Outliers are due to use of only Earth's crust composition
- Tested with success for other planets, Moon and asteroids
- Described by a Boltzmann distribution depending on the distance to the protosun
- Predicts high initial content of hydrogen
- Earth currently has about 4% by weight of hydrogen.
- It is mainly combined as hydrides and partly dissolved into other phases

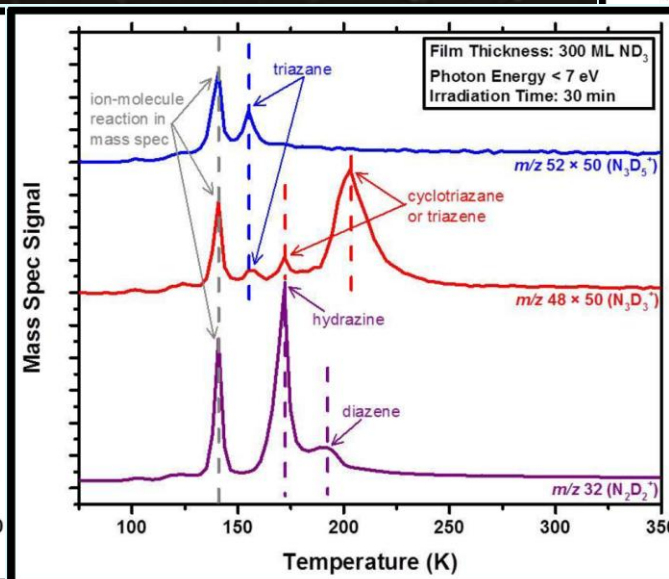
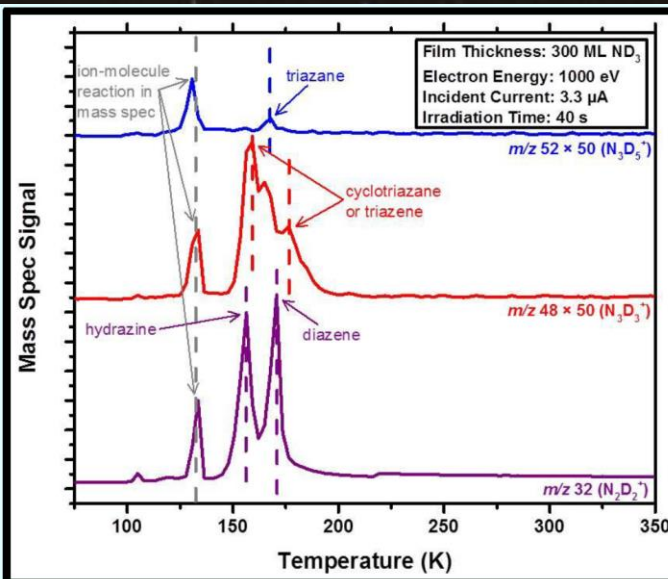
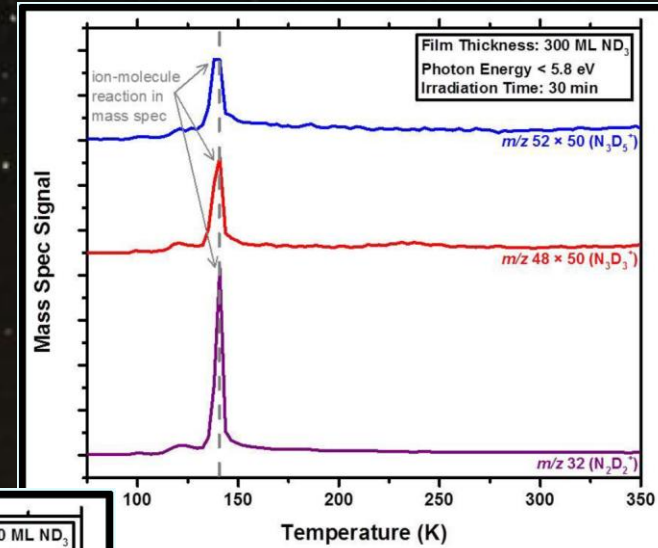
<http://arxiv.org/abs/1208.2909v2>

# Non-Ionizing UV (< 7 eV) Photochemistry of Cosmic Ice Analogs of Ammonia

Radiolysis involves electron excitation due to particle radiation in addition to all ionization

Photochemistry involves electron excitation without ionization

- reactions initiated by cations
- production of low-energy electron cascade
- non-uniform distribution of reaction intermediates, non-selective chemistry leading to multiple reaction products



We see production of N<sub>2</sub> and N<sub>3</sub> species with high-energy electrons and < 8 eV photons, but not with < 6 eV photons



**Islem Bouhali**  
**Soumaya Bezzaouia**  
**Mourad Telmini**

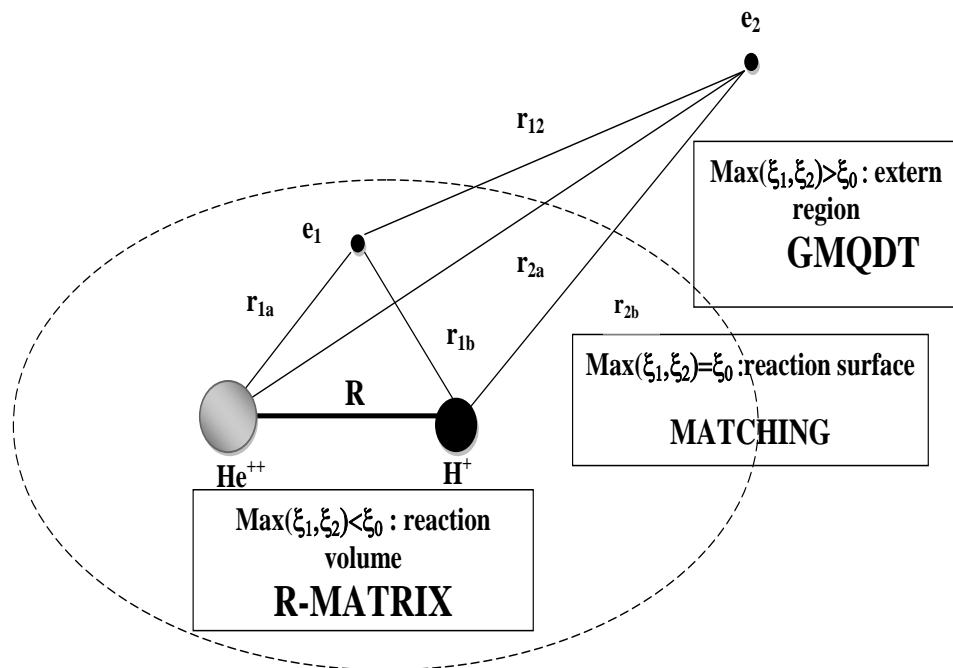


**Christian Jungen**

# **Theoretical study of Rydberg states of HeH<sup>+</sup> ion using the Halfium model**

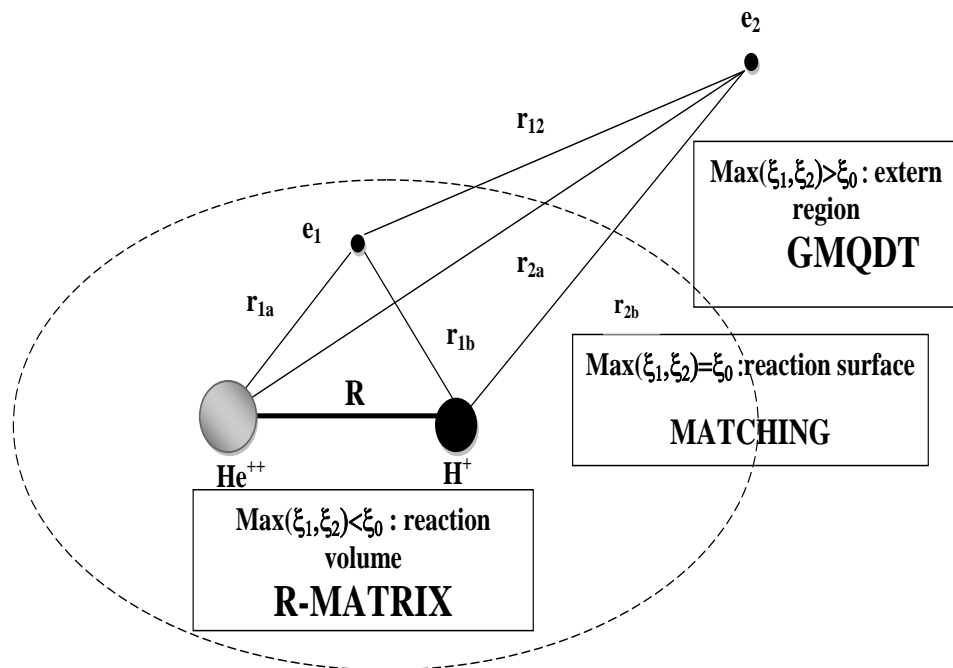
**Presented by: Islem Bouhali**

# HeH<sup>+</sup> molecular ion in Born-Oppenheimer approximation

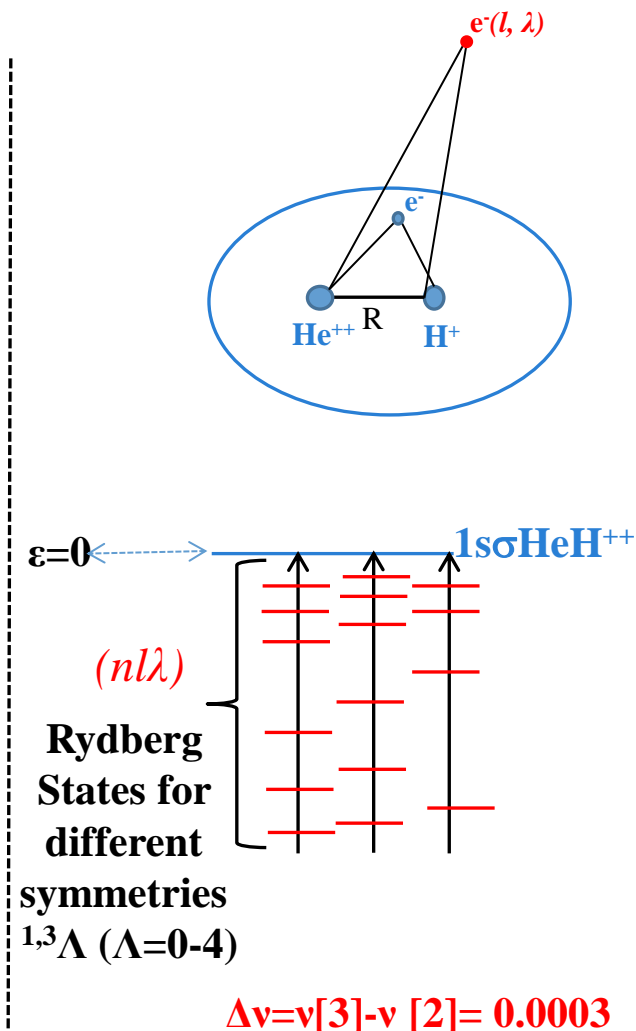


**Combination of the Variational  
 R-matrix method and  
 of the Generalized Multichannel  
 Quantum Defect Theory**

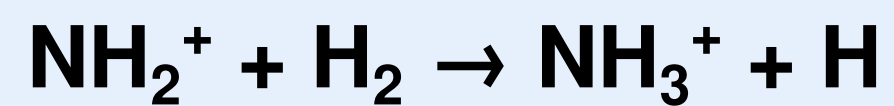
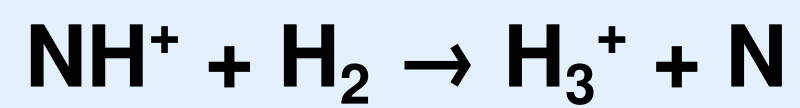
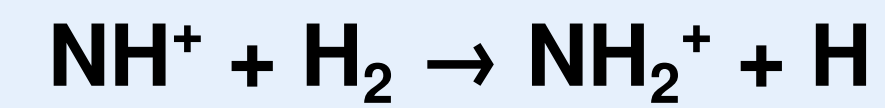
# HeH<sup>+</sup> molecular ion in Born-Oppenheimer approximation



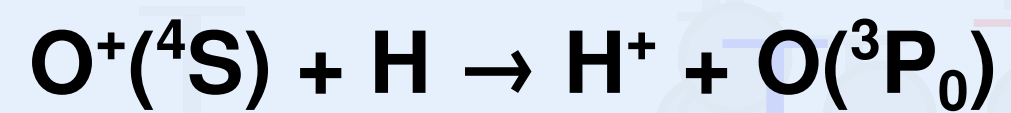
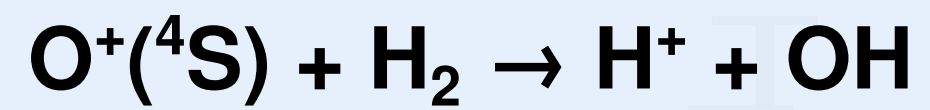
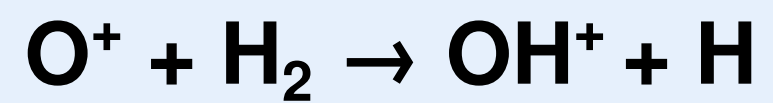
Combination of the Variational R-matrix method and of the Generalized Multichannel Quantum Defect Theory



- [1] I. Bouhali, S. Bezzaouia, M. Telmini and Ch. Jungen, EPJ Web of Conferences. 84 04004 (2015).  
 [2] I. Bouhali, S. Bezzaouia, M. Telmini and Ch. Jungen, Phys. Rev. A, 94, 022516 (2016).  
 [3] M. Jungen and Ch. Jungen, Mol. Phys. 113, 2333 (2015).



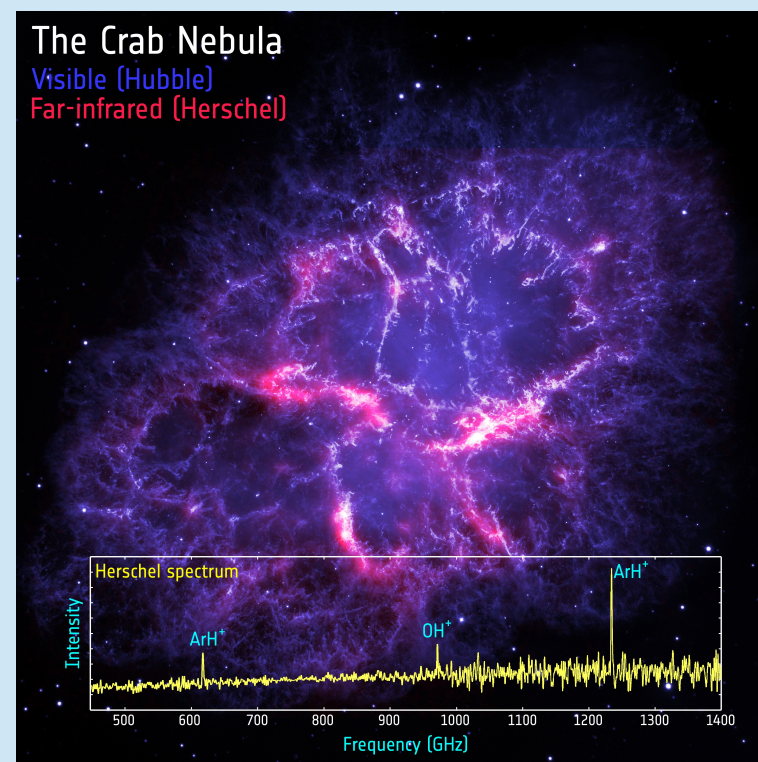
POSTER 21  
Štěpán Roučka



# An investigation of the argonium emission from the Crab Nebula

Felix Priestley, Mike Barlow, Serena Viti  
University College London

- Argonium ( $\text{ArH}^+$ ) discovered in emission in Crab Nebula by Barlow et al. (2013), followed by detection in absorption in ISM by Schilke et al. (2014) and towards extragalactic sources by Müller et al. (2015).
- Interstellar  $\text{ArH}^+$  requires low molecular hydrogen fraction to form, situation in Crab Nebula less clear due to X-ray synchrotron emission and probable high charged particle flux.
- Combination of photoionisation and photodissociation region modelling used to investigate molecular abundances in Crab Nebula knots/filaments, and compare predicted line emission to Herschel SPIRE FTS data.



# Poster 23: Formation of Solid H<sub>2</sub>-Bodies

H<sub>2</sub> Phase Transition + Gravity = Substellar H<sub>2</sub> Bodies

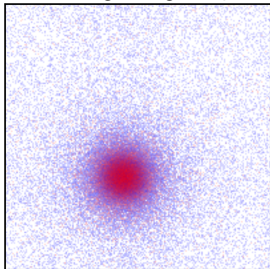
## Motivation

- Formation of solid H<sub>2</sub>
  - During star formation
  - In cometary knots
  - In cold disks
- Solid H<sub>2</sub> as dark baryons

## Conclusions

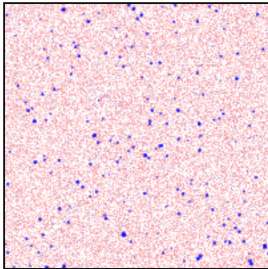
- Fluids in a phase transition
  - Always gravitationally unstable
  - Jeans length vanishes
- Phase transition + gravity:  
Gas → grains → planetoids

Ideal gas + gravity



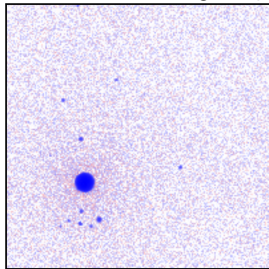
Formation of gaseous  
He-planetoid

Phase transition



Formation of solid  
H<sub>2</sub>-oligomers

Phase transition + gravity



Formation of solid  
H<sub>2</sub>-planetoid



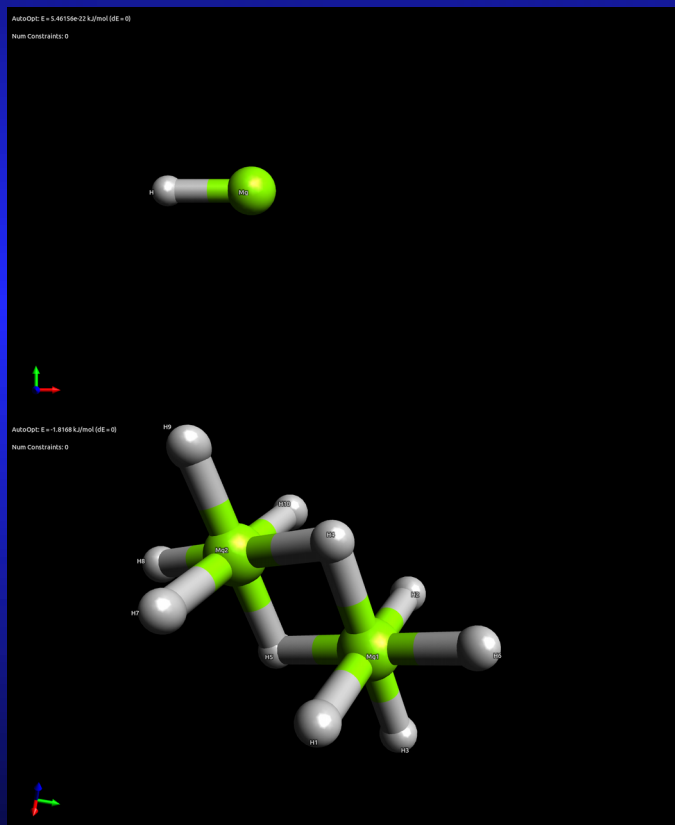
# MgH<sub>2</sub> in space and interaction with H

Carla Maria Coppola

Università degli Studi di Bari, Dipartimento di Chimica

Via Orabona 4, I-70126, Bari, Italy

carla.coppola@uniba.it



1- Thermochemistry

2- Electronic structure

3- Stability & chemical bonds



MgH<sub>2</sub> vs MgH  
in cold ISM  
(?)



UNIVERSITÀ  
DEGLI STUDI DI BARI  
ALDO MORO



UNIONE EUROPEA



·a·r·t·i·

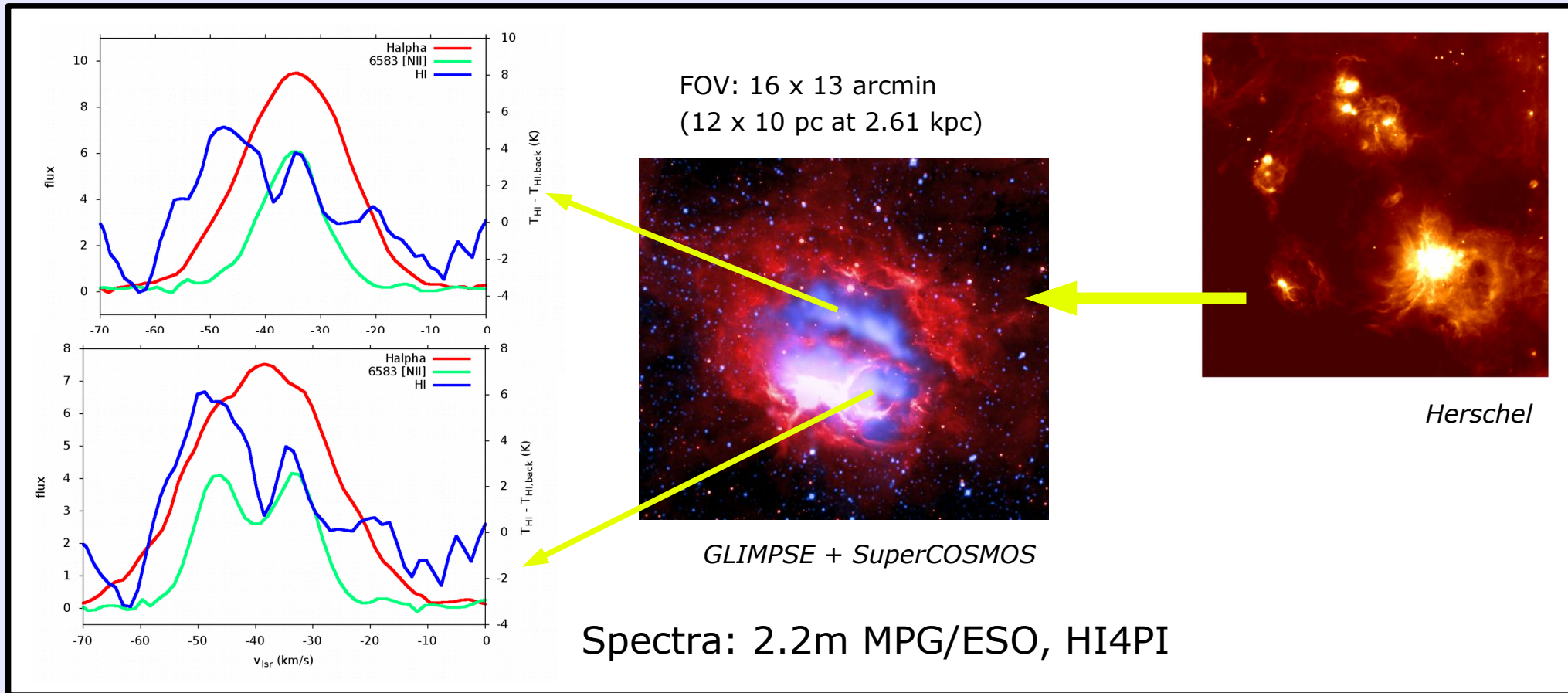
Agenzia regionale  
per la tecnologia  
e l'innovazione

# Optical observations of IR bubbles S73 and S74

**Soňa Ehlerová<sup>1</sup> & Lenka Zychová<sup>2</sup>**

<sup>1</sup>Astronomical Institute, Czech Academy of Sciences

<sup>2</sup>Faculty of Science, Masaryk University, Brno



# The Impetus project:

Using the supercomputer ABACUS for the HPC of Radiative Tables for accretion onto a galaxy Black Hole

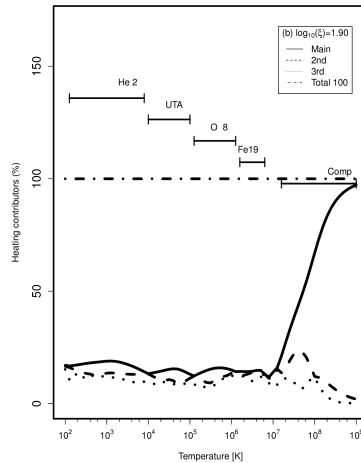
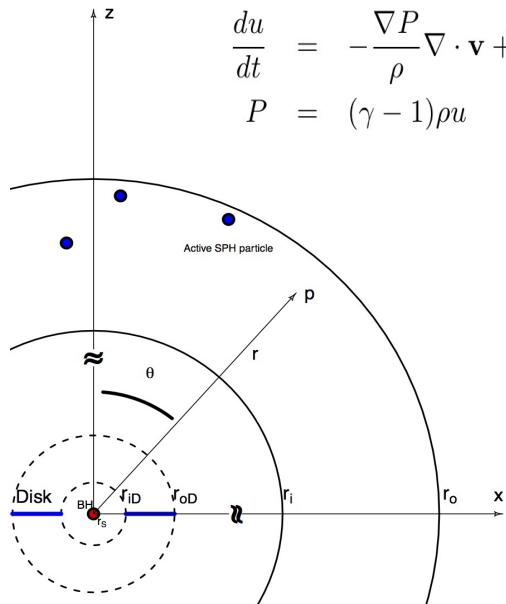
José M **Ramírez-Velasquez** (IVIC), Jaime Klapp (ININ), Ruslan Gabbasov (UAEH), Fidel Cruz (UAM-A), Leonardo Di G. Sigalotti (UAM-A)

$$\frac{d\rho}{dt} + \rho \nabla \cdot \mathbf{v} = 0$$

$$\frac{d\mathbf{v}}{dt} = -\frac{\nabla P}{\rho} + \mathbf{g}^{grav} + \mathbf{g}^{rad}$$

$$\frac{du}{dt} = -\frac{\nabla P}{\rho} \nabla \cdot \mathbf{v} + \frac{\Gamma(u, \rho) - \Lambda(u, \rho)}{\rho}$$

$$P = (\gamma - 1)\rho u$$



Hydride Toolbox 2016

SMBH Disk Model:

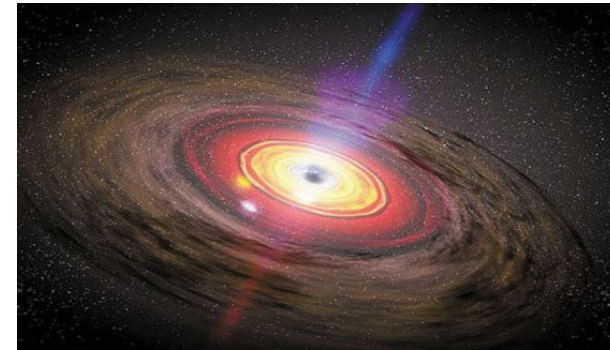
$$M_{BH} = 10^8 \text{ solar masses}$$

$$R_{ID} = 3R_{Sch} = 3 \cdot 2GM_{BH}/c^2$$

$$R_{oD} = 10R_{Sch}$$

$$T = 1.3 \times 10^5 - 4 \times 10^5 \text{ K}$$

Initial SED for the disk



ABACUS: Laboratorio de Matemáticas Aplicadas y Cómputo  
de Alto Rendimiento del Departamento de Matemáticas

INICIO
ACERCA DE ABACUS
INFRAESTRUCTURA
CONVOCATORIA 2016
RESULTADOS
CONTACTO

**Impetus: Photoionisation + SPH, numerical simulations of astrophysical objects**

Digital Tables of the accretion of matter onto SMBH in the center of galaxies

Calculation	File Name	Size (MB)
I	New_DB_SED1_1_short.gz	47
II	New_DB_SED1_2_short.gz	47
III	New_DB_SED1_3_short.gz	47
IV	New_DB_SED2_1_short.gz	47
V	New_DB_SED2_2_short.gz	47
VI	New_DB_SED2_3_short.gz	47

CARRETERA MÉXICO-TOLUCA KM. 38.5 OCOYOACAC, ESTADO DE MÉXICO

<http://www.abacus.cinvestav.mx/impetus>

# Ortho-para ratio of H<sub>2</sub>O in molecular clouds: development of enrichment techniques to investigate the role of cold grains

T. Putaud, X. Michaut, M. Bertin, G. Féraud, R. Dupuy, P. Jeseck, L. Philippe, J.-H. Fillion and D. Lis

## Objectives

### Orion Nebula



Density  
Temperature  
Photon Flux

Crédit : Spitzer-Nasa

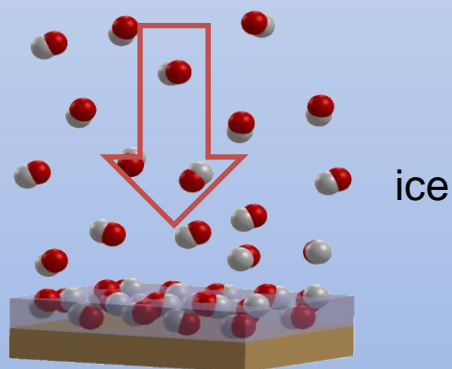
X. Michaut  
D. Lis  
M. Gerin  
J. Goicoechea ICCM  
B. Godard  
F. Le Petit

## Feasibility studies

Ice sample preparation  
Enriched in ortho H<sub>2</sub>O:  
- by optical pumping



- with magnetic lenses:

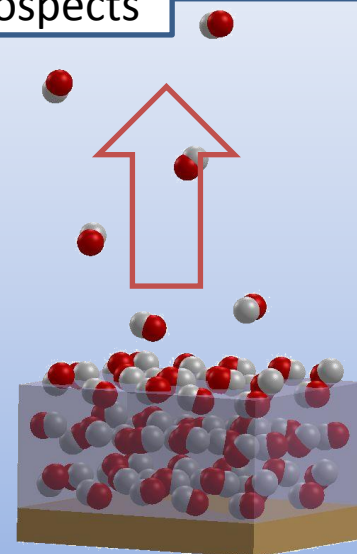


substrate T < 20 K

## Prospects



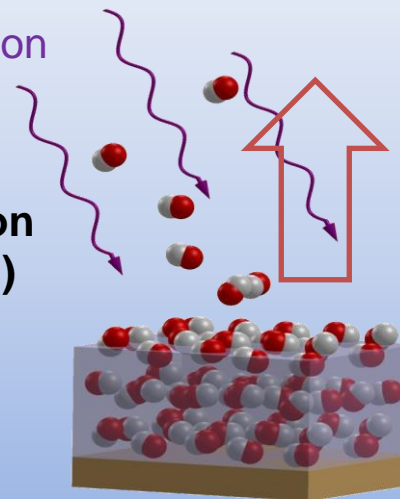
thermal  
desorption



VUV radiation

UV desorption  
(non thermal)

SPICES 2



# COMPLETE HYDROGENATION OF A PAH CATION

S. Cazaux<sup>1,2</sup>, L. Boschman<sup>1,3</sup>, N. Rougeau<sup>4</sup>, G. Reitsma<sup>3</sup>, R. Hoekstra<sup>3,5</sup>, D. Teillet-Billy<sup>4</sup>, S. Morisset<sup>4</sup>, M. Spaans<sup>1</sup>, and T. Schlathölter<sup>3</sup>

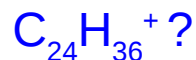
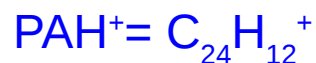
(1) Kapteyn Astronomical Institute, University of Groningen, P.O. Box 800, NL 9700 AV Groningen, The Netherlands.

(2) Leiden Observatory, Leiden University, P.O. Box 9513, NL 2300 RA Leiden, The Netherlands.

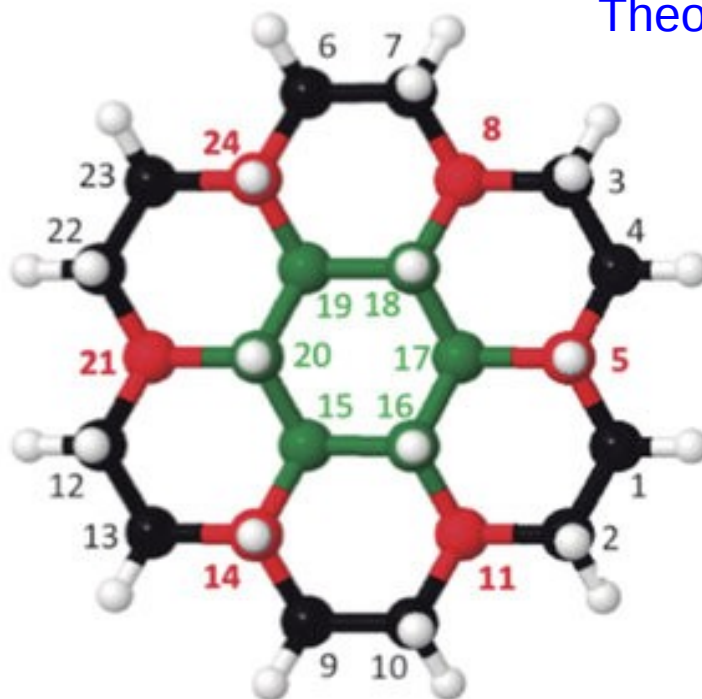
(3) Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 4, 9747AG Groningen, The Netherlands.

(4) Institut des Sciences Moléculaires d'Orsay, CNRS, Univ Paris-Sud, Université Paris Saclay, F-91405 Orsay, France.

Astrophysical context



+5H +11H et +17H more stable ?



Theoretical Calculations / Experiments

Binding energies ?

Hydrogenation barriers ?

Hydrogenation sequence ?