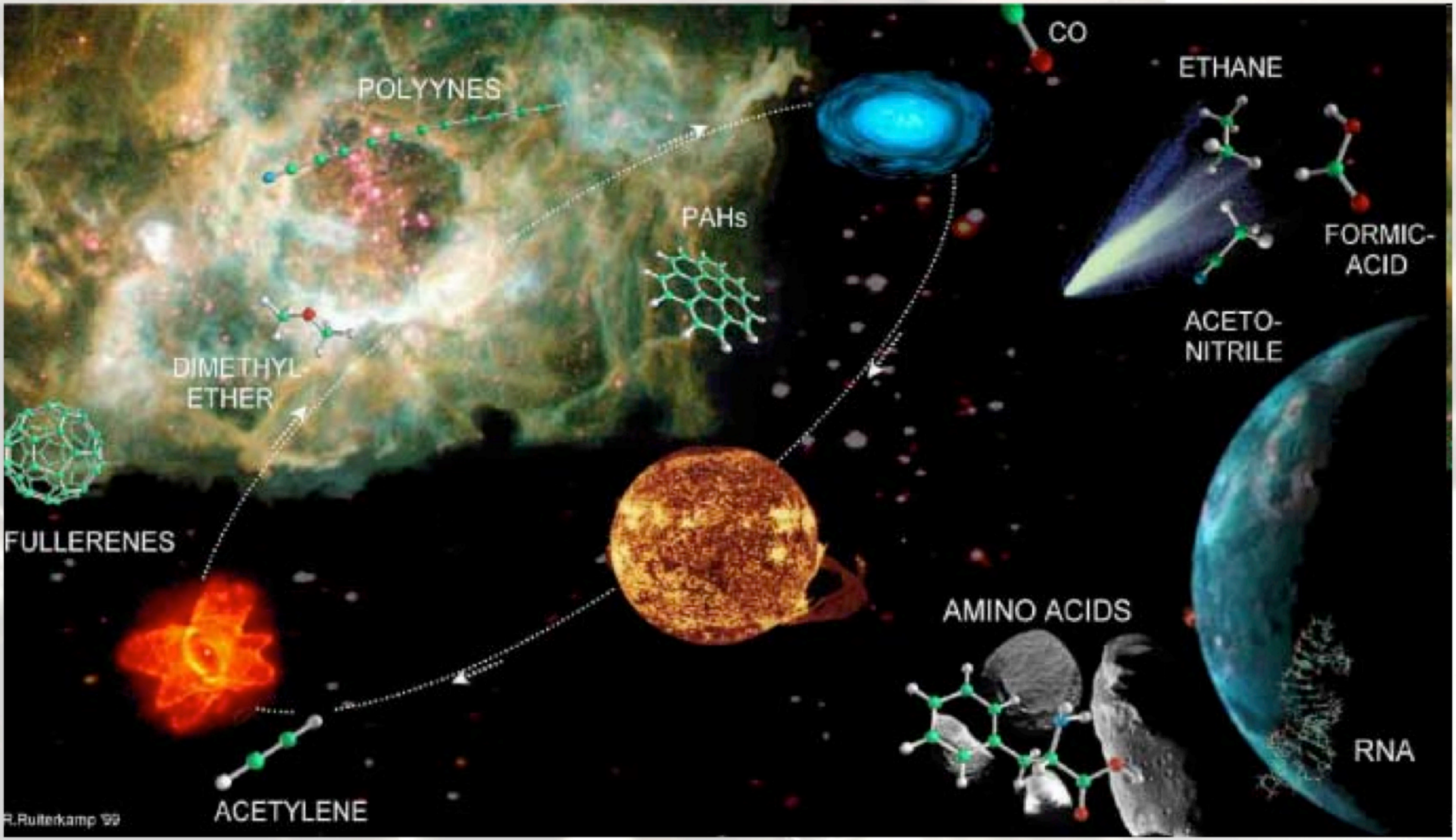
OASIS: an Optical Absorption Setup for Ice Spectroscopy

Complex molecules embedded in an interstellar ice analogue

S.H. Cuylle, J. Bouwman, E.D. Tenenbaum,
L.J. Allamandola, H. Linnartz
Leiden Observatory, University of Leiden

The interstellar cycle of matter



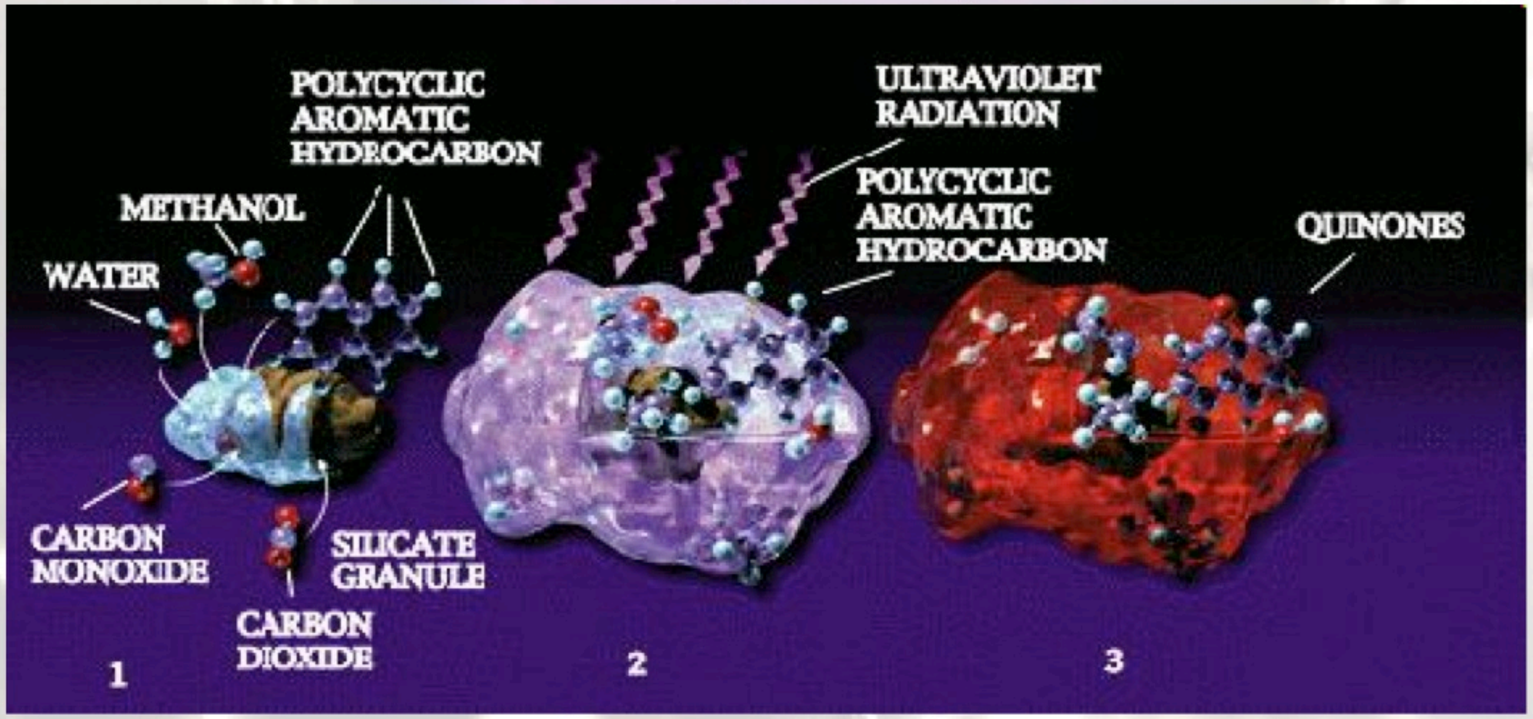
Interstellar ice

Molecules freeze out on dust grains as cloud condenses

→ H_2O, CO, CO_2, CH_4, CH_3OH, NH_3, …

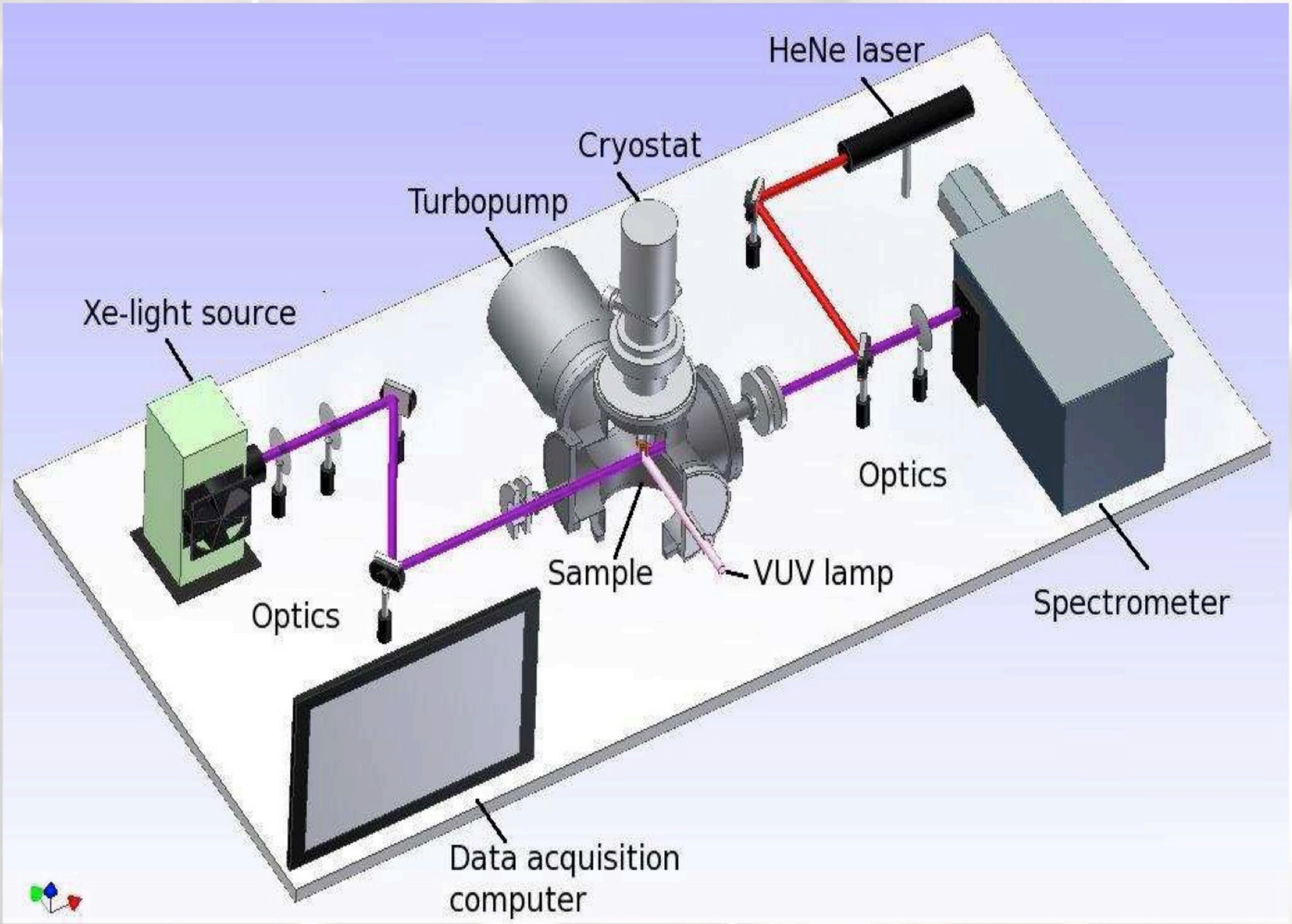
Less volatile species - PAH's and other complex molecules – will also accrete.

→ Ice acts as molecule reservoir and catalyst: VUV irradiation introduces a very complex chemistry.



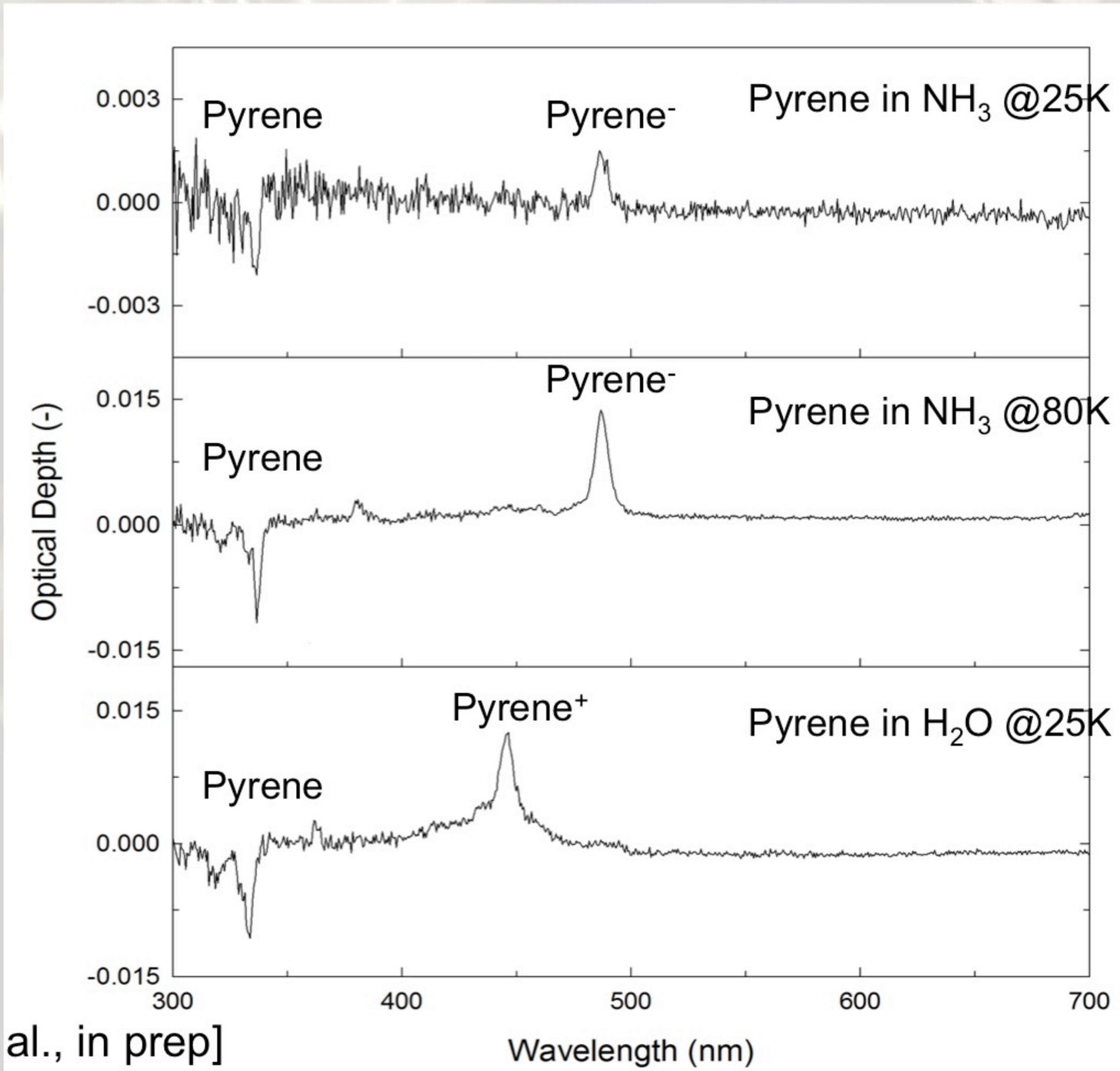
[Fig. courtesy Allamandola],[Greenberg, 1974, 1987, 2000; Nuevo et al., 2011]

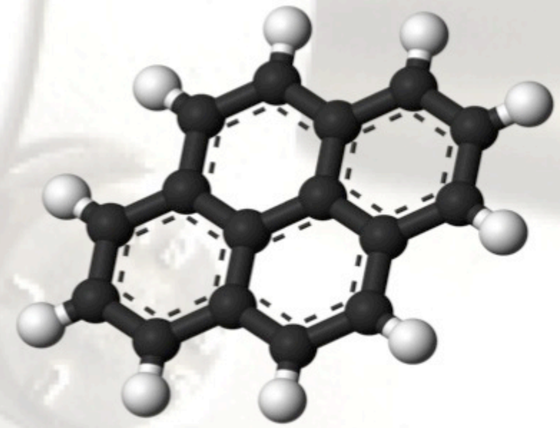
The OASIS setup



[Bouwman et al. 2009, 2010, 2011]

Dependency of photoproducts on temperature and matrix





[Tenenbaun et al., in prep]

LASSIE collaboration and training

- Leiden training event (may 2011)
  - Presentation skills
  - Outreach training
  - Personal skills development
- Astrochemistry course E. van Dishoeck
  - Obtain an overview of astrochemistry
- Collaboration with John Thrower (Aarhus university)
  - C_{60} in water ice
  - Increase knowledge of the mass spectrometer
- Industrial placement (2013)
- Scientific placement (2013)

Thank you for your attention!

Formation Routes of Interstellar Molecules through Surface Reactions at Low Temperatures

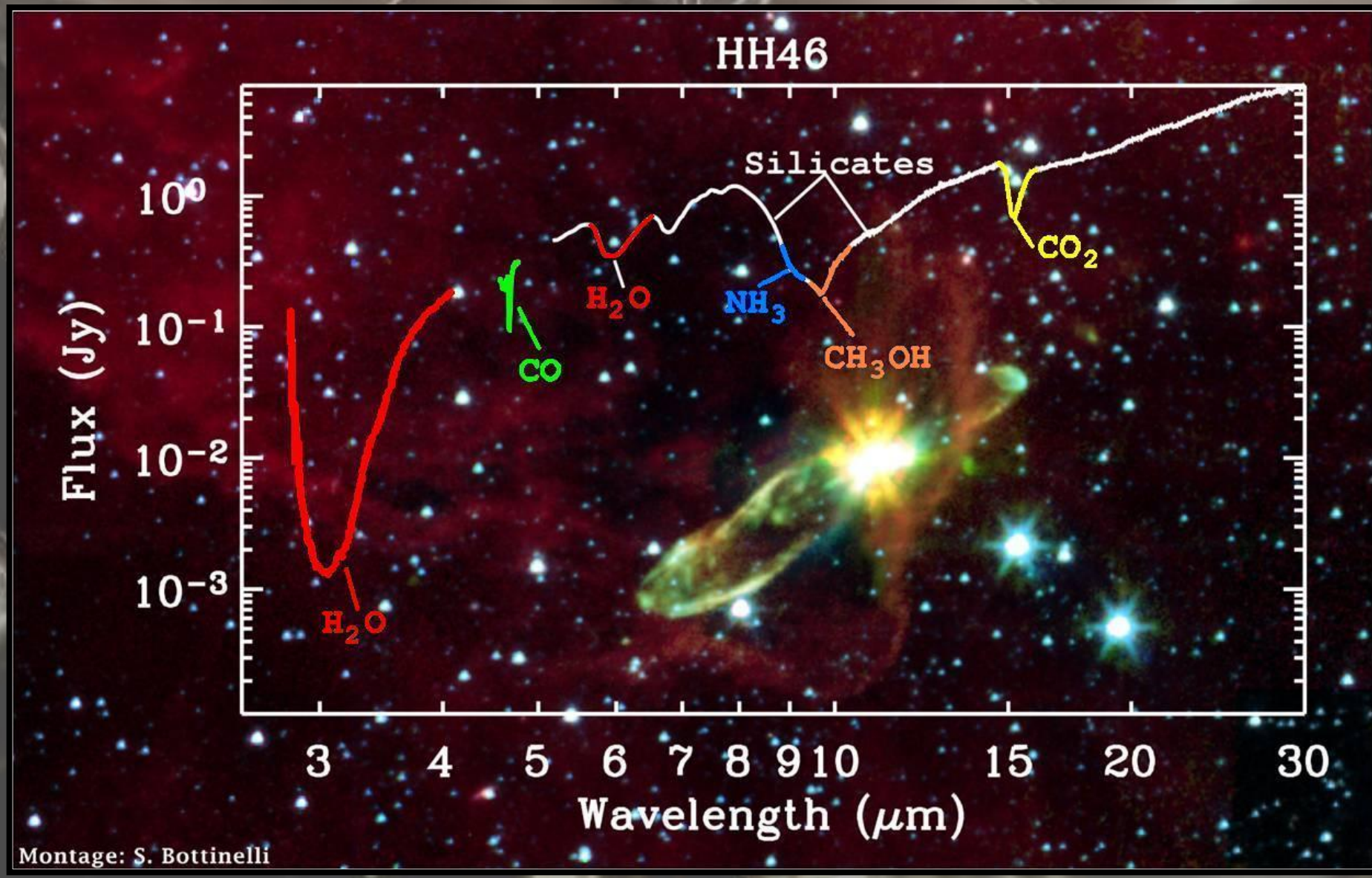
Gleb Fedoseev, Sergio Ioppolo, Herma Cuppen, Harold Linnartz

Sackler Laboratory for Astrophysics,
Leiden Observatory, University of Leiden, 2300 RA Leiden, NL

Paris, 14th of November

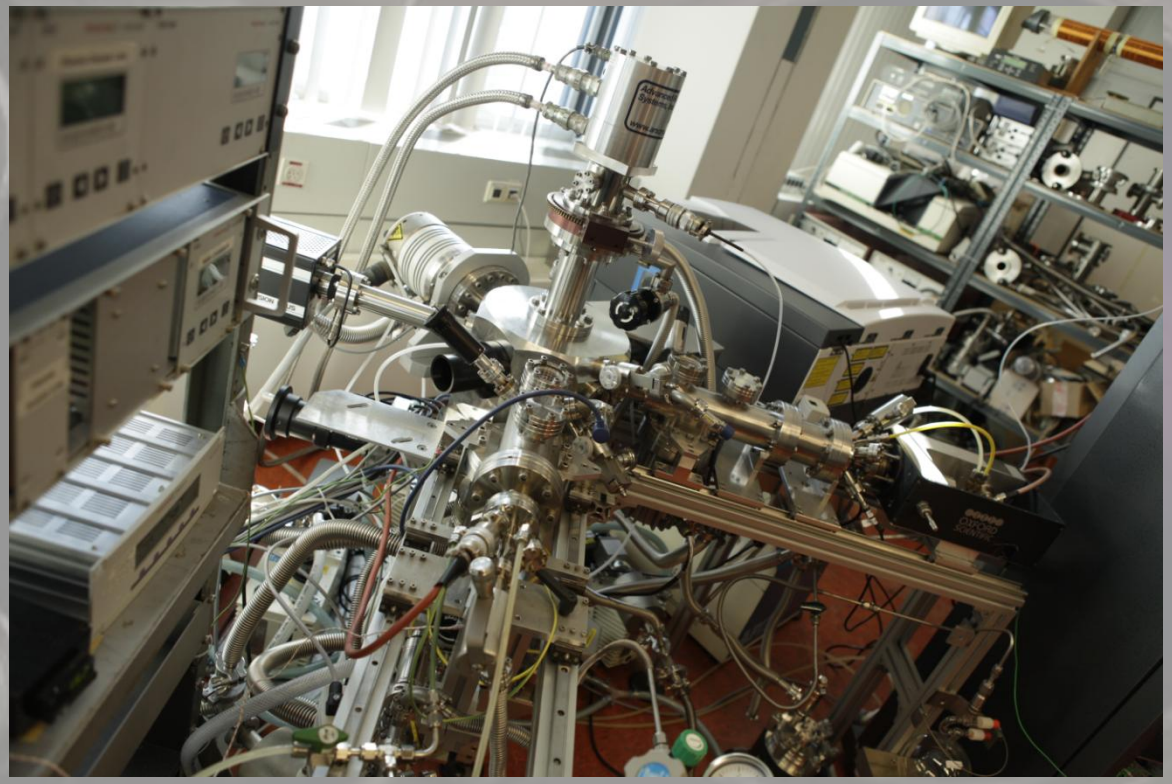
e-mail: fedoseev@strw.leidenuniv.nl

Interstellar Medium Has a Rich Chemistry



Analysis and Method

SURFRESIDE II Ultra High Vacuum (UHV) setup

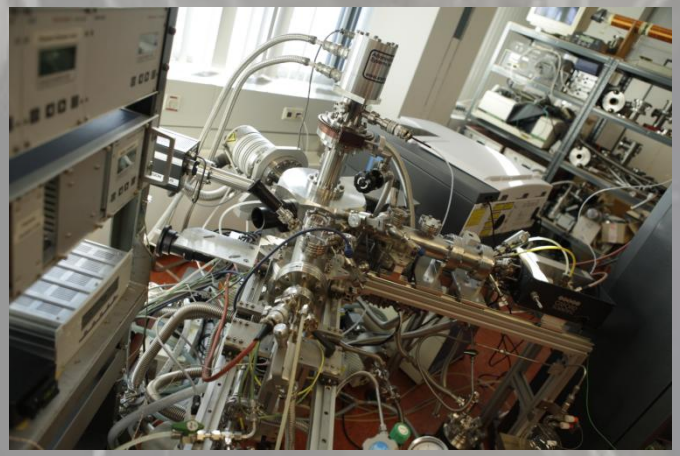


Pressure: ~ 10^{-10} mbar
Temperature: 12-300 K
Ice thicknesses: 10-100 ML

H - fluxes: $10^{12} – 10^{14}$ $cm^{-2}s^{-1}$
O-, N-, OH- fluxes: > 10^{12} $cm^{-2}s^{-1}$
Time: 3 – 5 hours

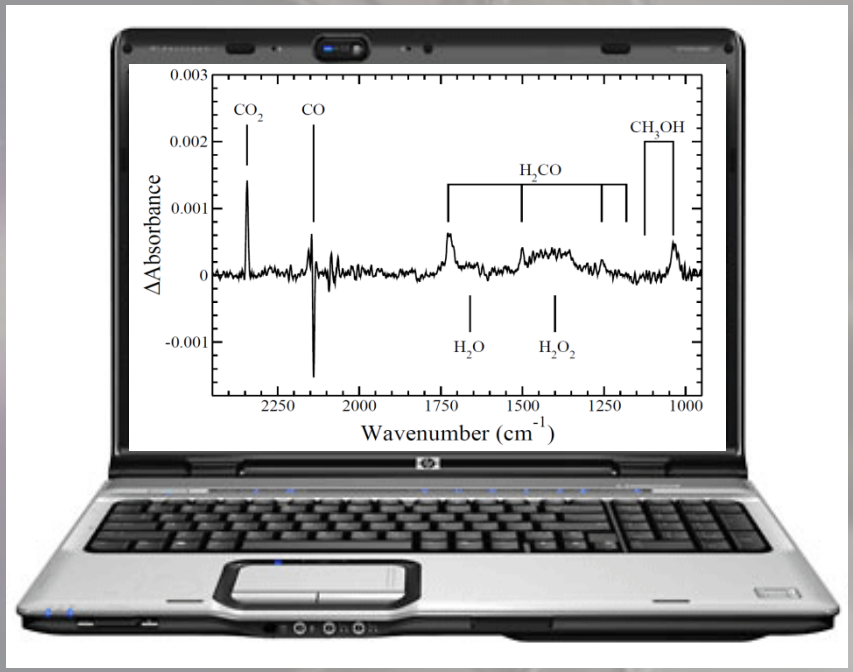
Analysis and Method

SURFRESIDE II UHV setup



Pressure: ~ 10^{-10} mbar
Temperature: 12-300 K
Ice thicknesses: 10-100 ML
H - fluxes: $10^{12} – 10^{14}$ $cm^{-2}s^{-1}$
O-, N-, OH- fluxes: > 10^{12} $cm^{-2}s^{-1}$

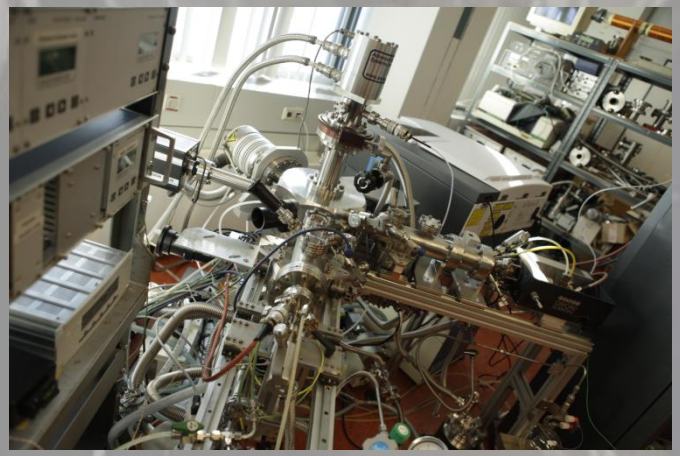
SURFRESIDE II has two complementary analytic tools



RAIRs
- in situ analysis
- does not damage the ice
- provides kinetic information
- low sensitivity

Analysis and Method

SURFRESIDE II UHV setup



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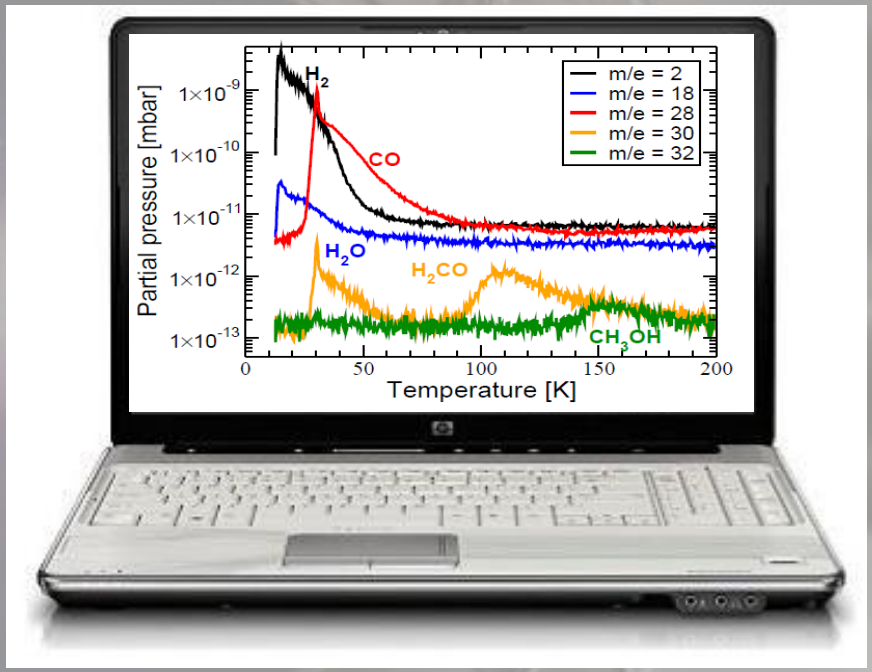
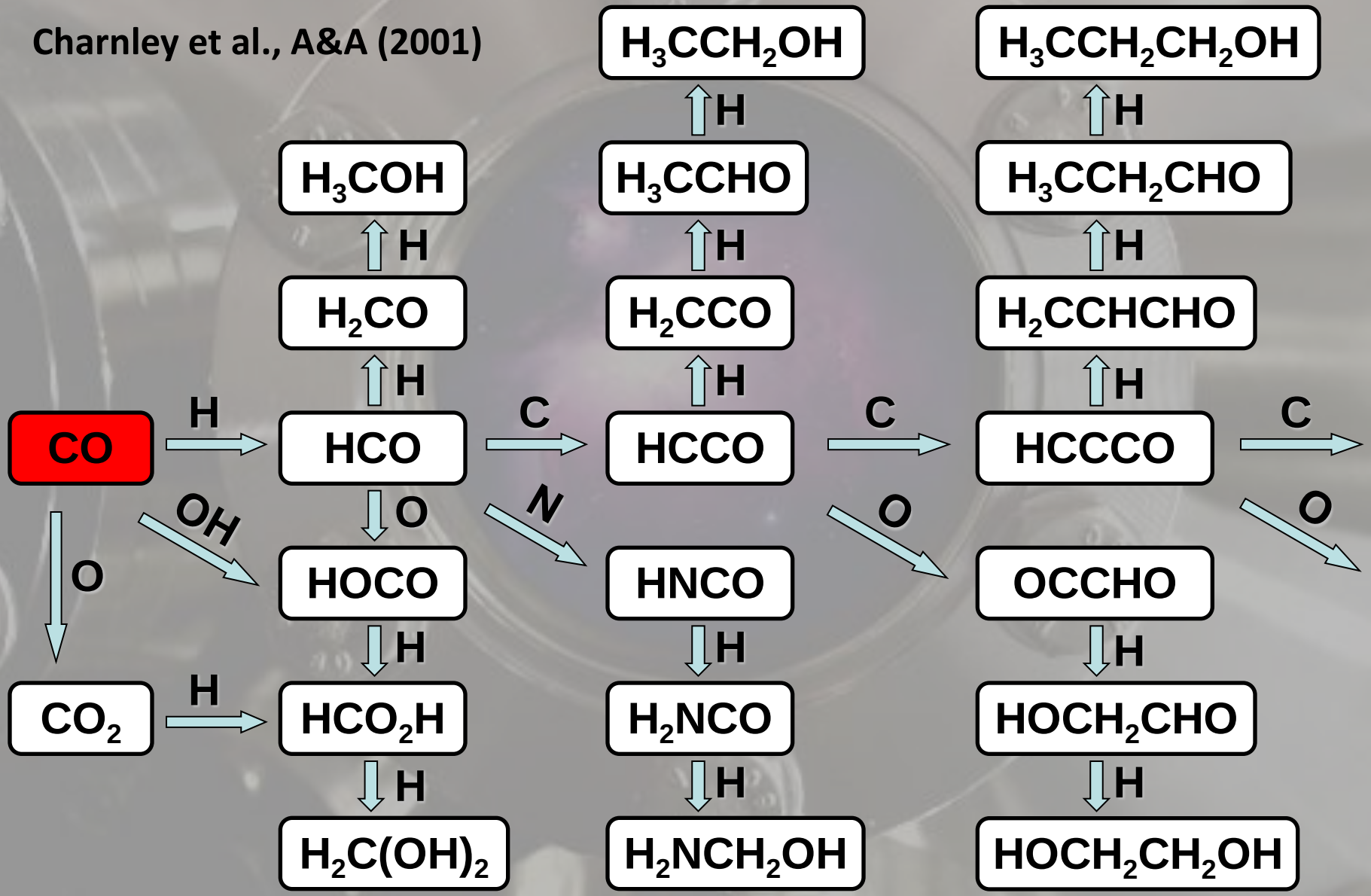
SURFRESIDE II has two complementary analytic tools



QMS
- in situ gas phase composition analysis
- damages the ice
- high sensitivity

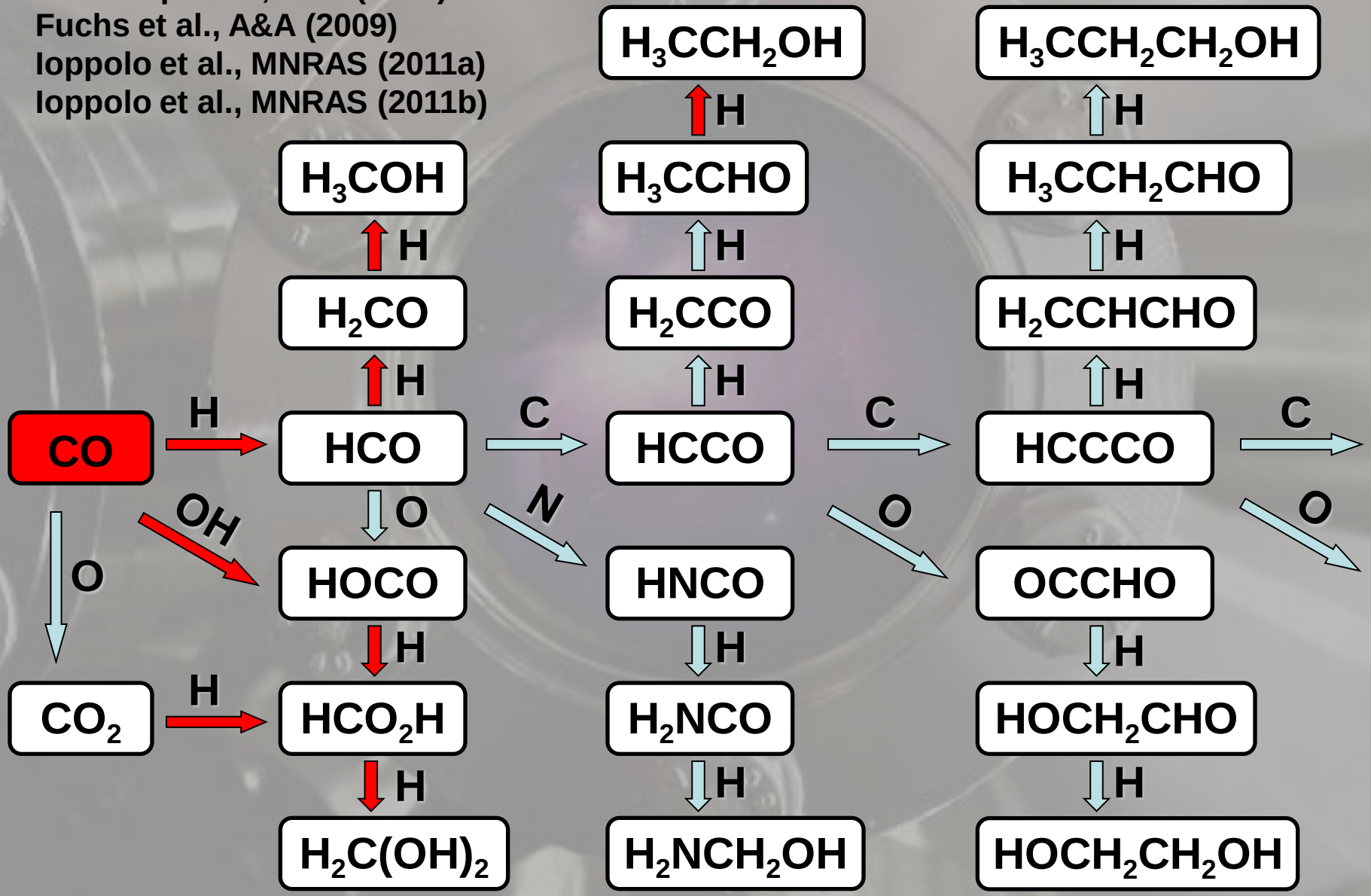
Research Project Goals

Charnley et al., A&A (2001)



Research Project Goals

Bisschop et al., A&A (2007)
Fuchs et al., A&A (2009)
Ioppolo et al., MNRAS (2011a)
Ioppolo et al., MNRAS (2011b)



Training and Research Progress

Skills Required:

Experience with UHV setups:
- design
- construction
- use

Acquisition of a solid background in astrochemistry

Personal Skills:
- presentation
- time management
- project management

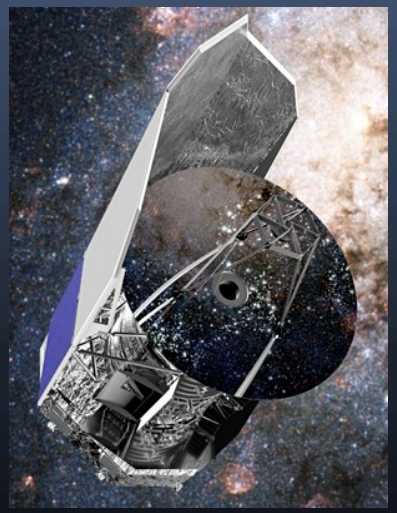
Workshops and trainings

- Laboratory work
- LASSIE Research Placement
- LASSIE Industrial Placement

- Lorentz Centre Workshops
- Lectures on "Astrochemistry", "Star and Planet formation"

- LASSIE Training events
- Daily supervisor assist

Tracing CO in Young Stellar Objects with Herschel-HIFI



Irene San José García

E. F. van Dishoeck, F. van der Tak,
L. E. Kristensen, J.C. Mottram

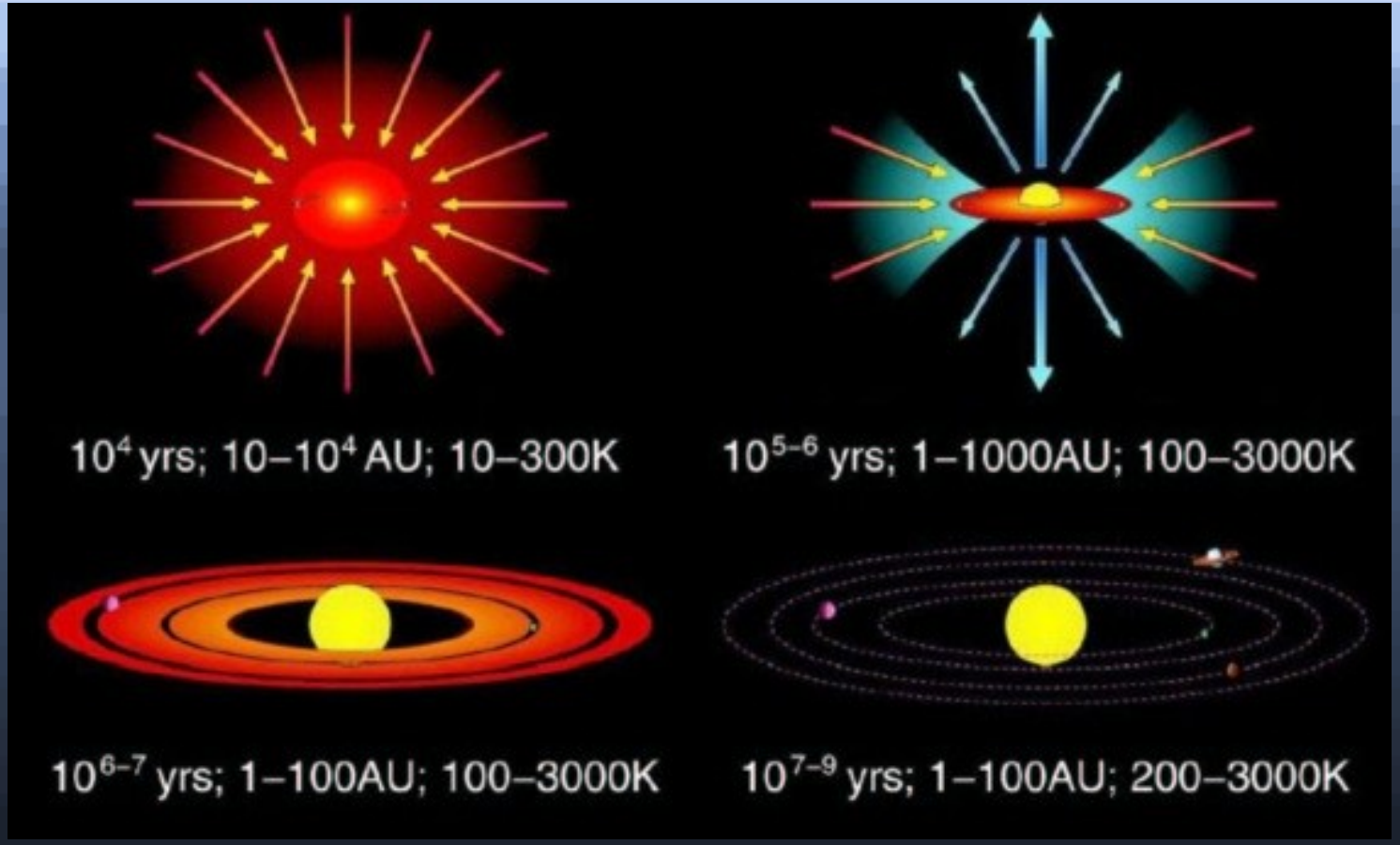
***Leiden Observatory**, University of Leiden, 2300 RA Leiden, NL*

PhD starting date: January 2011

sanjose@strw.leidenuniv.nl

More information: **http://www.strw.leidenuniv.nl/WISH/**

How stars form...



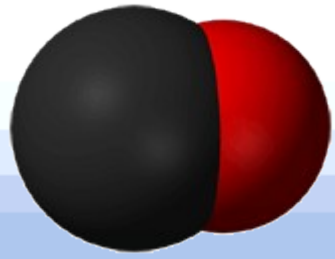
Scenario for low-mass star-forming regions.

From low- to high-mass protostars



- Most of the studies focussed either on low-mass or high-mass star-forming regions.
- Goal: Uniform picture of the star formation without mass boundaries.

CO as a diagnostic



- Present along the entire protostar system:
  - Probe the different components of the protostellar environment.
  - Observed in all the young stellar objects.
- Provide a reference to determine abundance of other complex molecules like water.

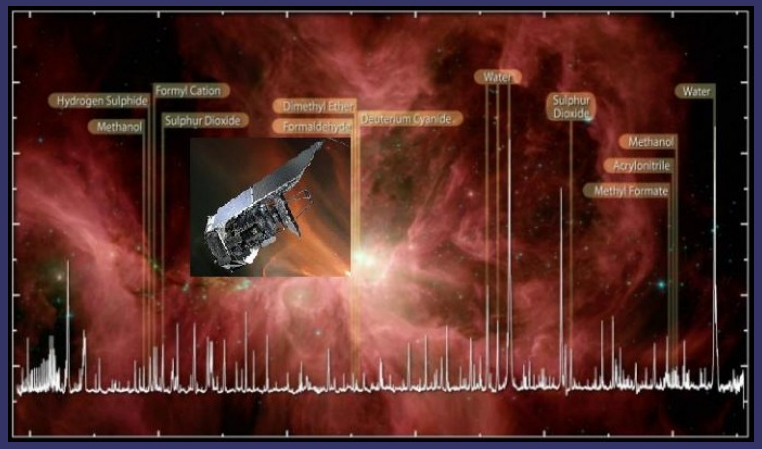
Observations

- **WISH**: *Water In Star-forming regions with Herschel*.
- Large guarantee *Herschel* key program.
- Tracing H_2O and other important molecules, like CO, along ~80 different young stellar objects.

- James Clerk Maxwell Telescope observations:
  - Complementing *Herschel* data.
  - Characterizing the CO ladder.

LASSIE OPPORTUNITIES

- **LASSIE training in Leiden, May 2011.** Time management, outreach, presentation skill, ...
- **“Astrochemistry Course”** by **E. F. van Dishoeck. T**eaching assistant of the course
- **IAU symposium 280:”The molecular universe”**, Spain. Poster presented.



- “**Astrosurf**” in Edinburgh, August 2011. Poster presented.
- **Observations at the JCMT in Hawaii,** August 2011. **PI of the project.**
- “**IRAM 30m summer school**”, Spain. September 2011. Lectures, observations and presentation.

- “**Young Astronomers' Meeting**”, tomorrow. Presenting a talk.
- Future scientific emplacements: **2013**
- **Active and friendly Network!**

Report at Midterm Review Meeting

Paris, November 2011

Anna Clemens, PhD student, LASSIE ESR

Department of Applied Physics, Chalmers University of Technology, Gothenburg, Sweden

Project: Physical processes and chemical transformations in and on icy grains

Start: May 2011

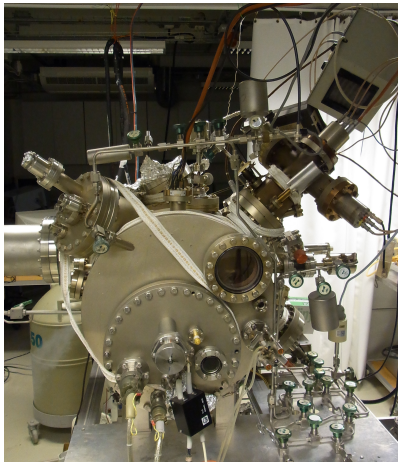
Supervision: Dinko Chakarov (first supervisor, LASSIE PI)
Henrik Grönbeck, Lars Hellberg (co-supervisor)

Research Project

- **Motivation:** Experimental Study of desorption mechanisms of ice deposited on model surfaces are of great importance to improve astrochemical models and explain astronomical observations

- **First project:** Photo- and thermal desorption of water ice from carbon nanostructures
  - ❖ Sizes of interstellar grains vary from Å to μm
  - ❖ Nanostructured carbon features have been observed [1]

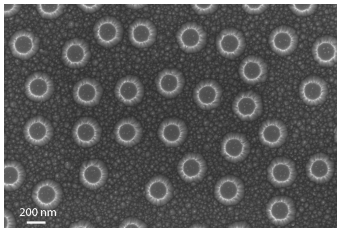
- **Experimental methods:**
  - Ultrahigh vacuum (UHV) conditions
  - Temperature: 100K
  - Ice deposition with controlled structure and thickness
  - Temperature programmed desorption (TPD) with quadrupole mass spectrometry detection of the product
  - Irradiation with continuous and pulsed light

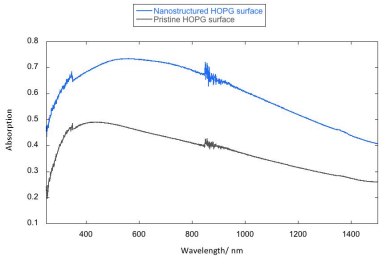


[1] Th. Henning et al., ASAP Conference Series, Vol. 309, 2004.

Research Project: First Results

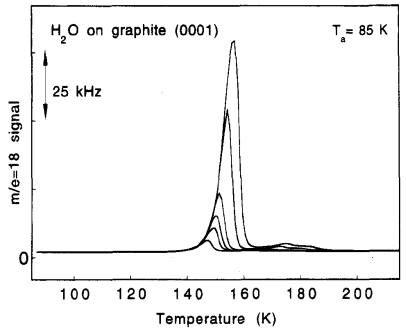
- Thermal desorption of H_2O deposited on nanostructured HOPG (highly oriented pyrolytic graphite)





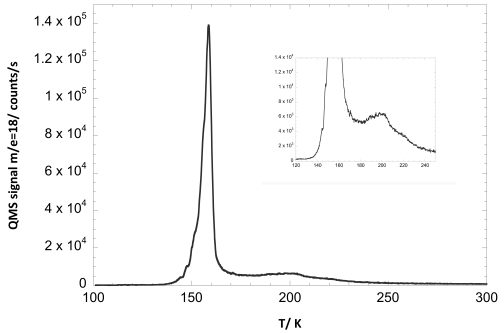
➢ **How is desorption influenced by a nanostructured surface?**

- Comparison of thermal desorption spectra with pristine HOPG surface



Left: TPD spectra of H_2O on bulk HOPG, heating rat: 2.5 K/s; coverage: 0.2 – 4ML; Modified from D. V. Chakarov *et al.*, *Langmuir* **1995**, *11*, 1201-1214.

Right: TPD spectrum of H_2O on nanostructured HOPG; heating rate: 1K/s, coverage: ca. 17ML.



➢ Additional peak at 190-220 K when using nanostructured surface

Trainings & Courses

Research skills and techniques:

- Training in ultrahigh vacuum techniques, Lars Hellberg, Dinko Chakarov
- Training in using cleanroom facilities for production of nanostructured surfaces, Department of Microtechnology and Nanoscience, Chalmers University

Courses and summer schools organized by LASSIE:

- "Astrochemistry" lectures, Ewine van Dishoeck, Leiden Observatory, May 2011
- Course in Presentation skills, Harold Linnartz, Leiden Observatory, May 2011
- Outreach training, Graphic Science, Leiden, May 2011
- Project and time management, Coenegracht training, Leiden, May 2011
- "Astrochemistry with ALMA", summer school, Bologna, June 2011

Courses organized by Chalmers:

- "Modern imaging, spectroscopy and diffraction techniques", credits: 7.5, September/October 2011
- "Ethics, Science and Society ", credits: 3, October/November 2011

Conferences and Workshops:

- "Negative Ions and Molecules in Astrophysics", Chalmers/Göteborg University, August 2011
- "AstroSurf" conference, Heriot-Watt University, Edinburgh, August/September 2011

Hydrogen atom diffusion on the surface of interstellar ices

Bethmini Senevirathne

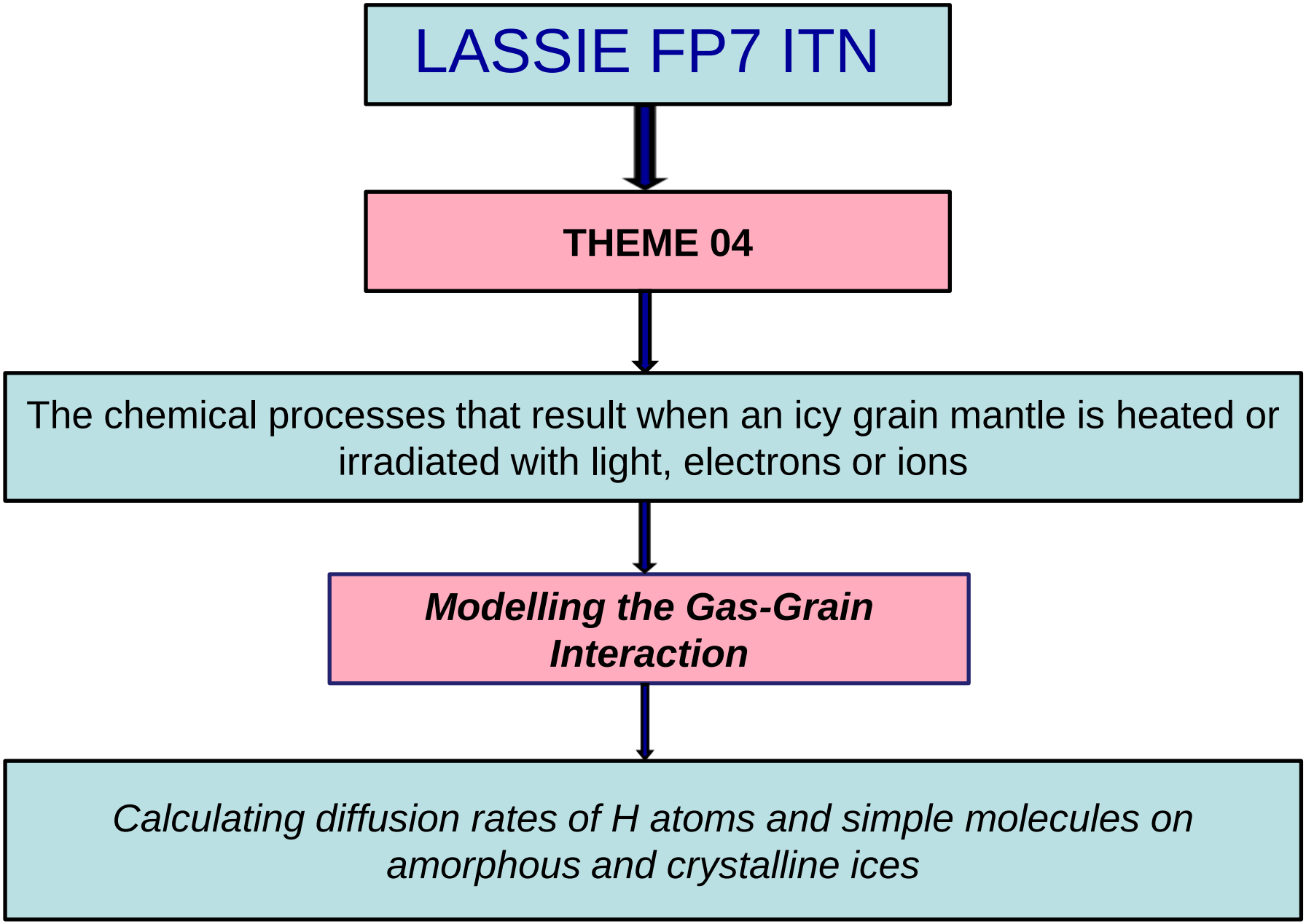
University of Gothenburg, Sweden

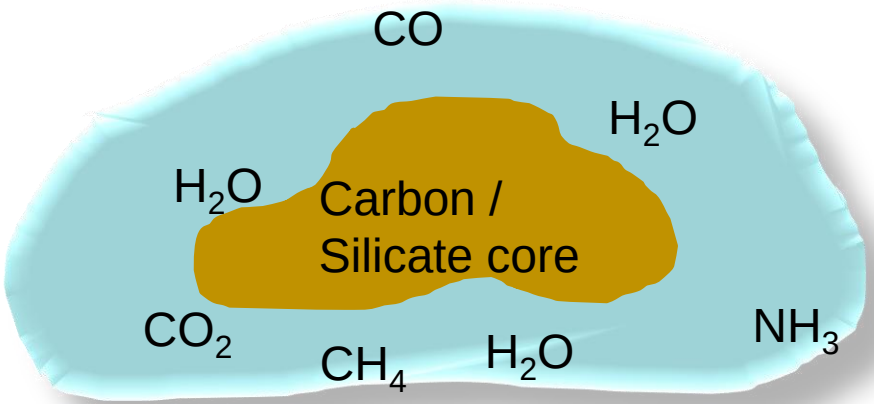
Prof. Gunnar Nyman

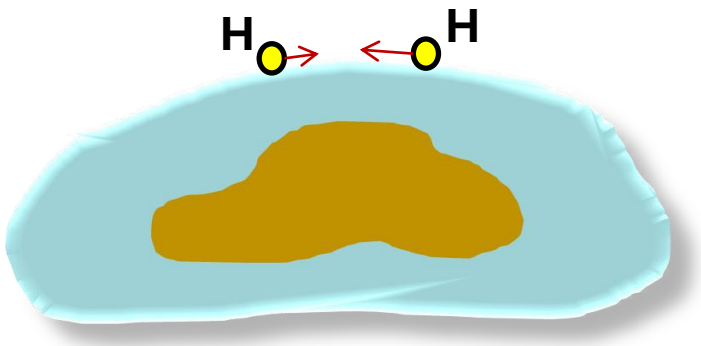
University of Gothenburg, Sweden

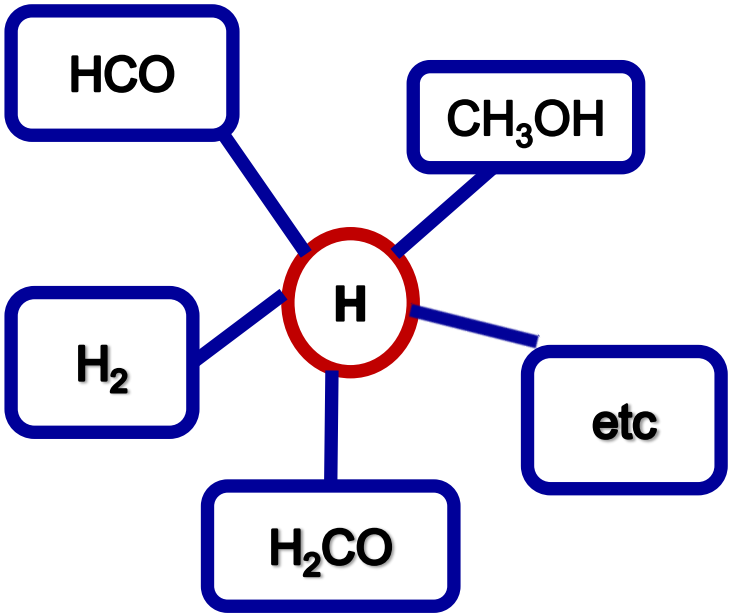
Dr. Stefan Andersson

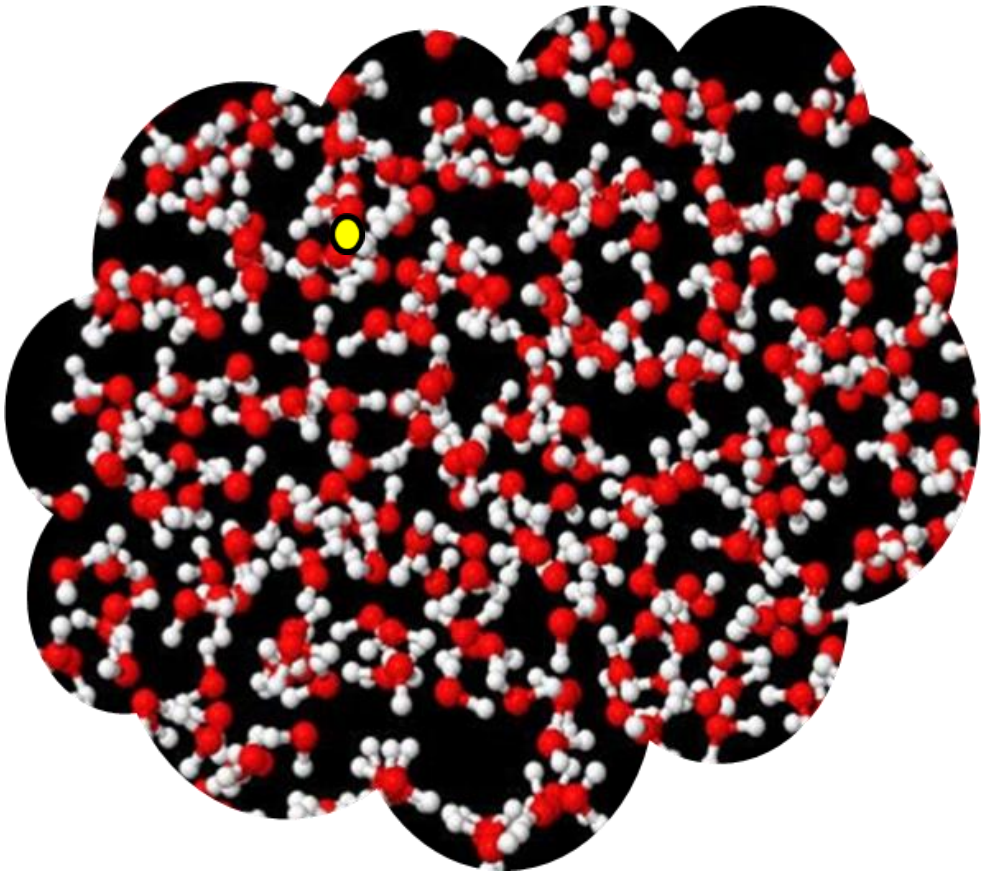
SINTEF Materials and Chemistry, Norway


LASSIE FP7 ITN
THEME 04
The chemical processes that result when an icy grain mantle is heated or irradiated with light, electrons or ions
Modelling the Gas-Grain Interaction
Calculating diffusion rates of H atoms and simple molecules on amorphous and crystalline ices

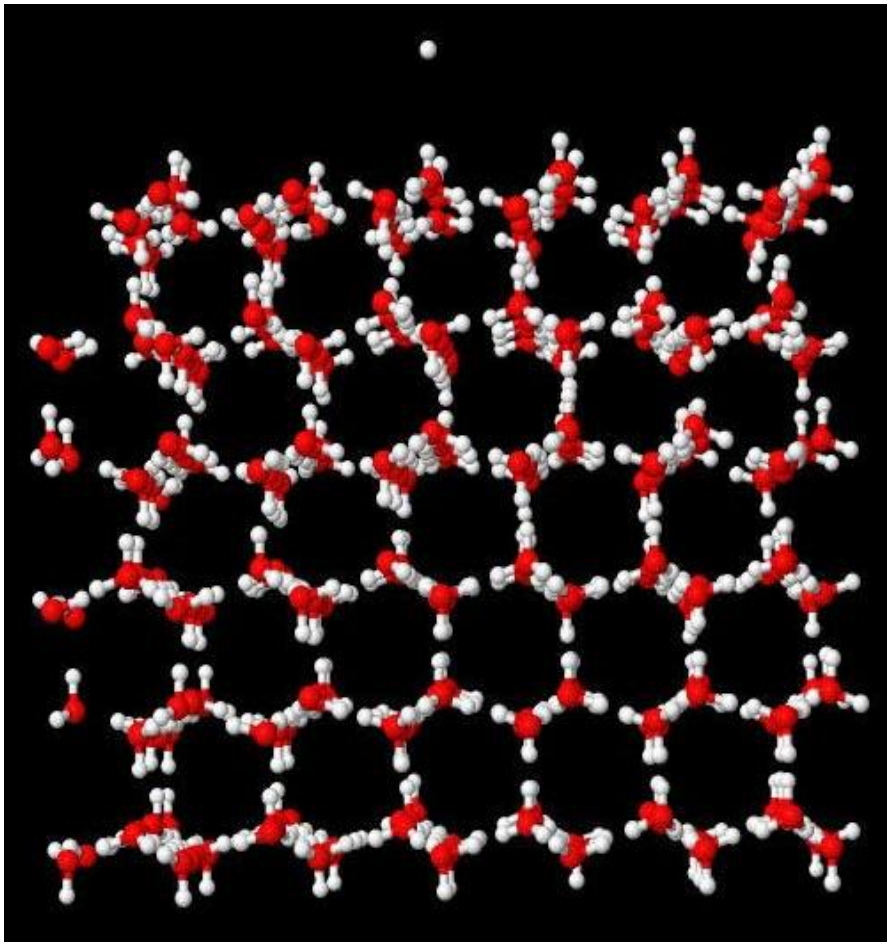

CO
H_2O
H_2O
Carbon /
Silicate core
CO_2
CH_4
H_2O
NH_3

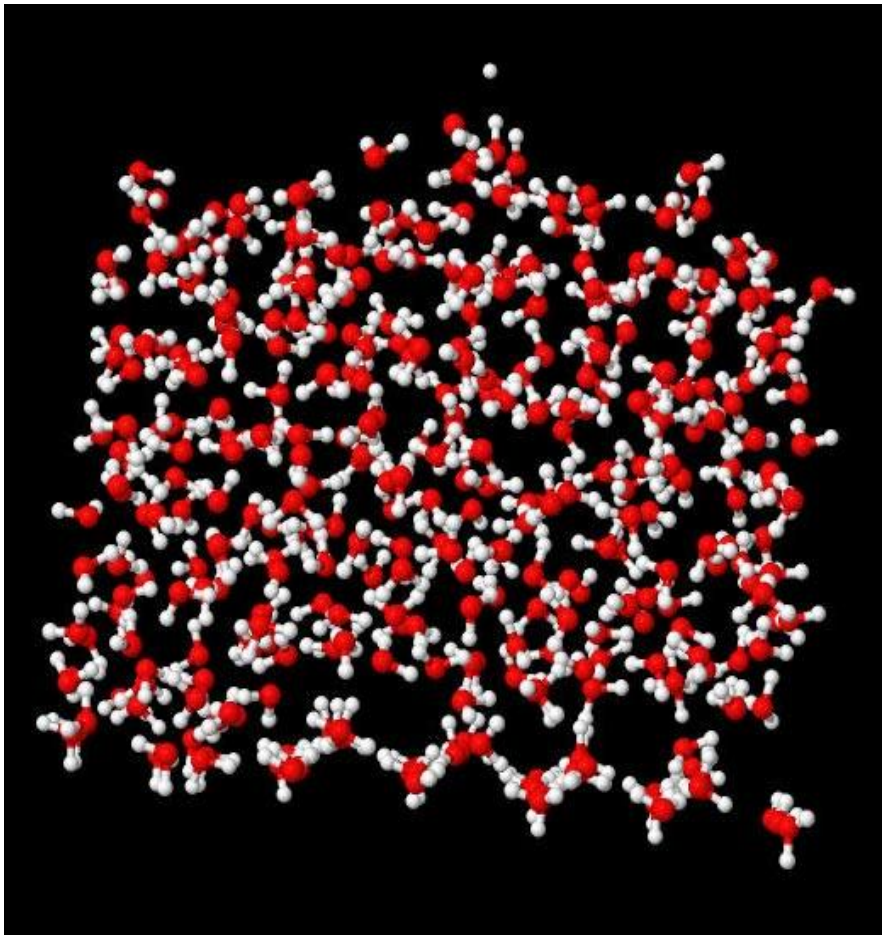

H
H


HCO
CH_3OH
H
H_2
etc
H_2CO



Ice structures: H atom diffusion on the surface of crystalline water ice and amorphous solid water

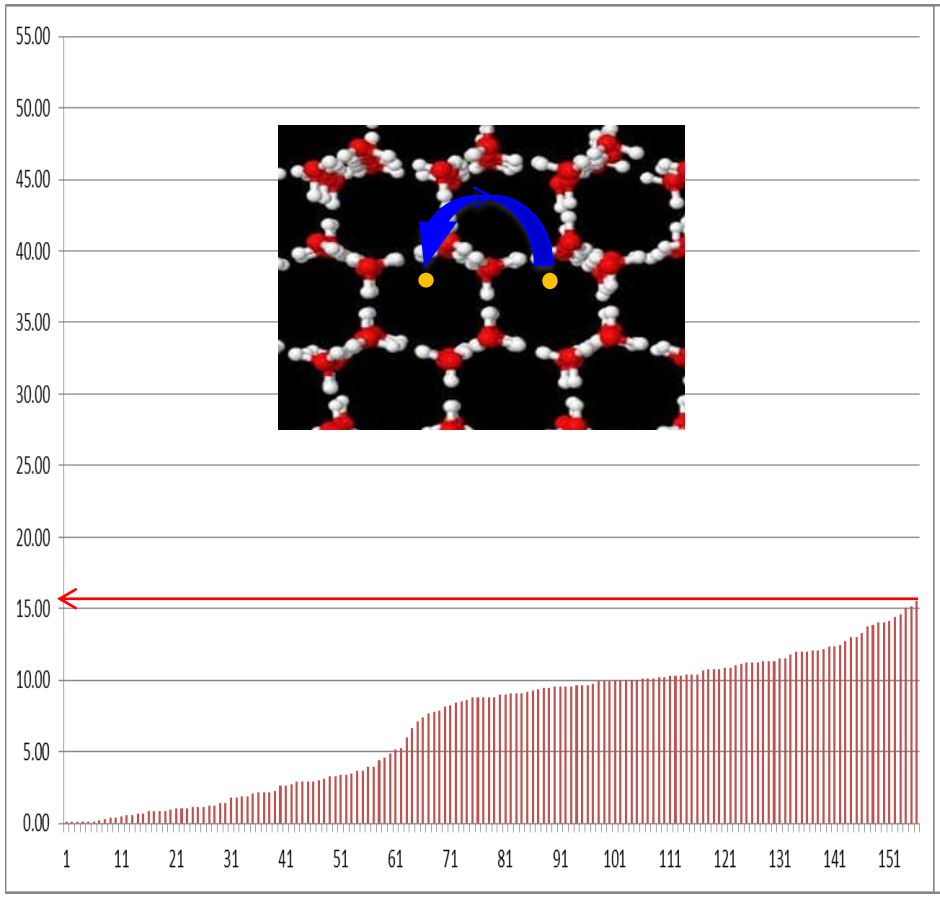




Andersson, S. *et a*l, 2006, *JCP*, 124, 064715

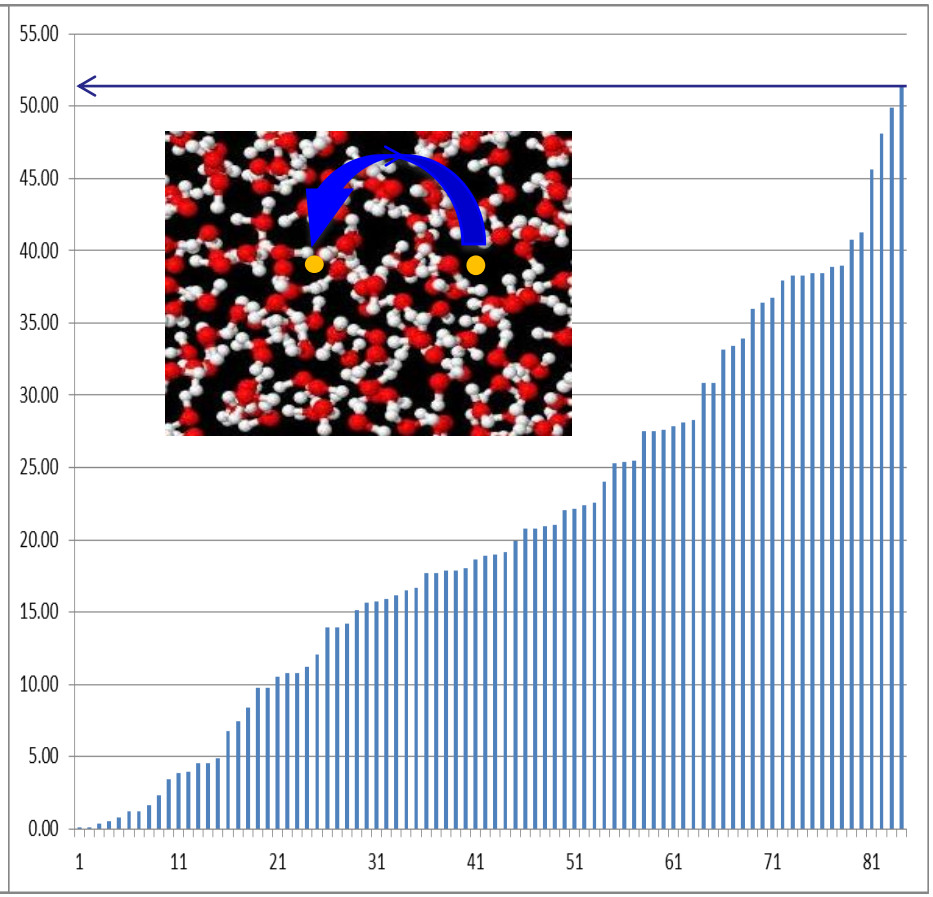
Results: Comparison between the activation energy

Crystalline ice



Activation energy (meV)

Amorphous ice



Activation energy (meV)

B. Senevirathne, S. Andersson, G. Nyman, In preparation.

Future goals …

- Calculate **diffusion coefficients** for H atom diffusion on the surface of amorphous ice and crystalline ice.
- Deuterium diffusion on the surface of water ices.
- H,D diffusion inside ice.
- H_2, HD, D_2 diffusion on the surface and inside ice.

Training

Summer schools and Workshops:

- Astrochemistry lectures: Prof. dr. E.F. van Dishoeck, May 17-26 2011 in Leiden, Netherland.
- International Summer School: Astrochemistry with ALMA June 13-17 2011 Location: Bologna (Italy)
- Workshop: Challenges in Modelling the Reaction Chemistry of Interstellar Dust: Sept. 19-24 2011 Leiden, Netherland.

Subject courses:

- Numerical and Mathematical methods for Chemist
- General Chemistry
- Physical Chemistry
- The interstellar Medium and Star Formation

Training

Teaching skills:

- Teaching and learning in Higher Education
- Lab assistant: Laboratory of Physical Chemistry
  - ❖Molecular spectroscopy (Experimental)
  - ❖Vapour pressure and vaporization enthalpy (Experimental)
  - ❖Quantum Chemistry using HyperChem (Computer lab)

Academic writing skills:

- English for Academic Purposes

Computer Programming skills:

- Fortran 77, Fortran 90, Perl,Octave, Python, Matlab

Training

Research discussions:

- Gunnar Nyman - Main supervisor: ~3 times per week
- Stefan Andersson - Supervisor: ~Once per two weeks via e-mail, skype conferences
- Per-Ola Norrby – Examiner: ~Once per week
- Colleagues:

    Dylan Drake-Wilhelm (LASSIE ER)

    Hua-Gen Yu

    Sergey Antipov

    Magnus Gustafsson

    Jens Poulsen

Thank you

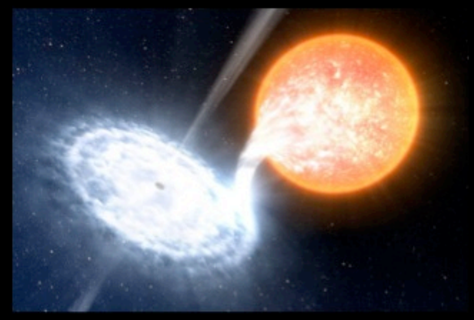
Experimental studies of surface reactions relevant to astrochemistry

Fabrizio Puletti

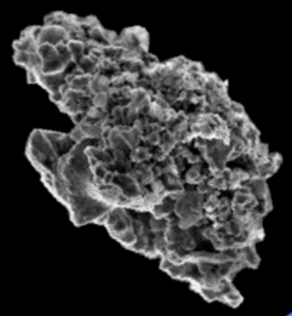
Supervisor: Dr Wendy Brown

Chemistry Department, University College London

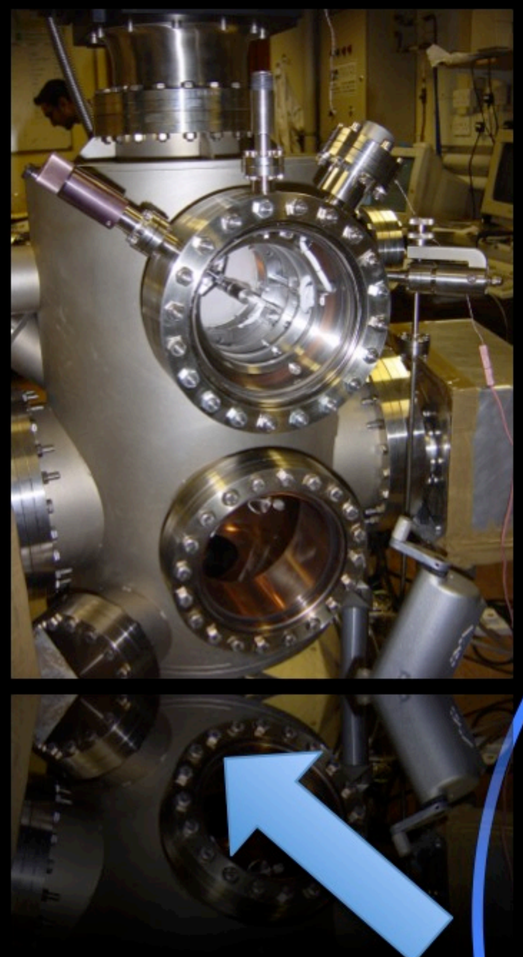
Space is full of stuff....



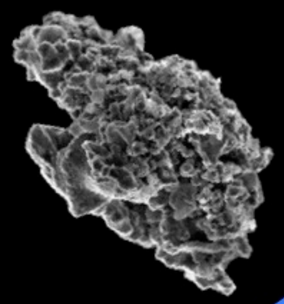
H H_2 H_2O CO CO_2 PAH HC_7N HCO OCS CH_3COOH **ISM** OCS SO_2 H_2S



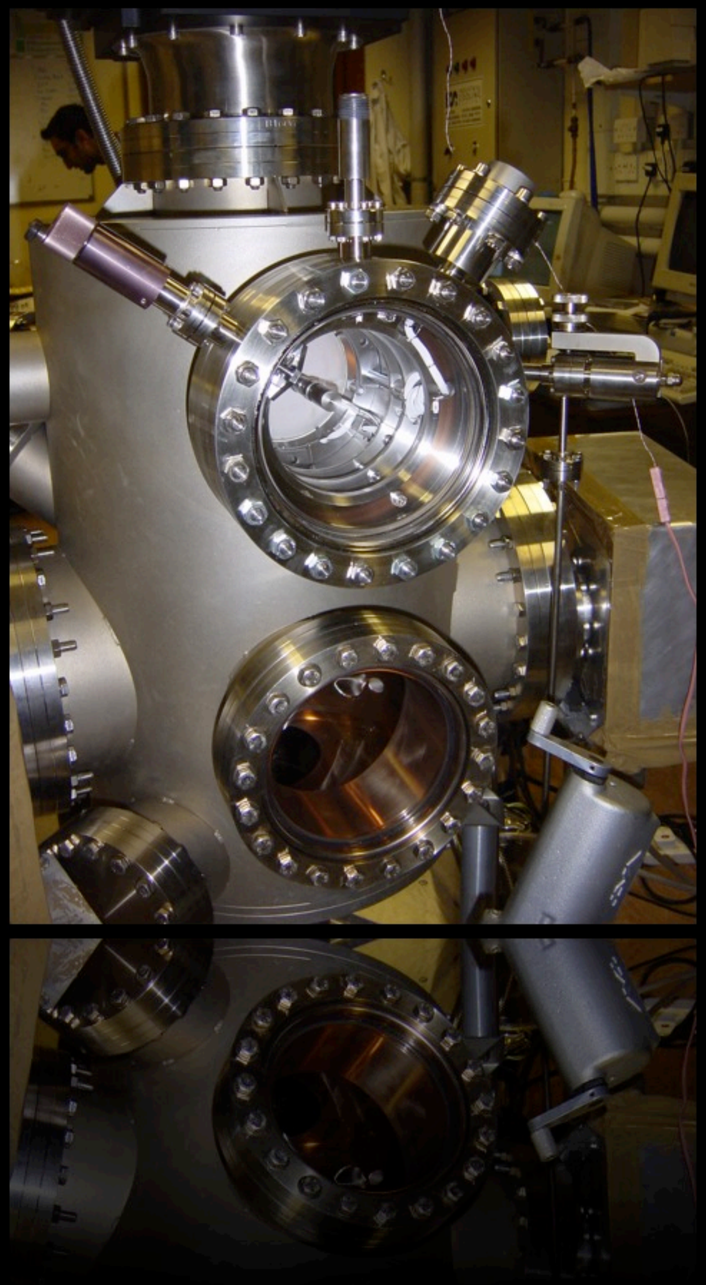
Potential approaches



H H_2
H_2O
HCO
OCS
CO
CO_2
PAH
HC_7N
CH_3COOH
ISM
OCS SO_2
H_2S



Experimental setup

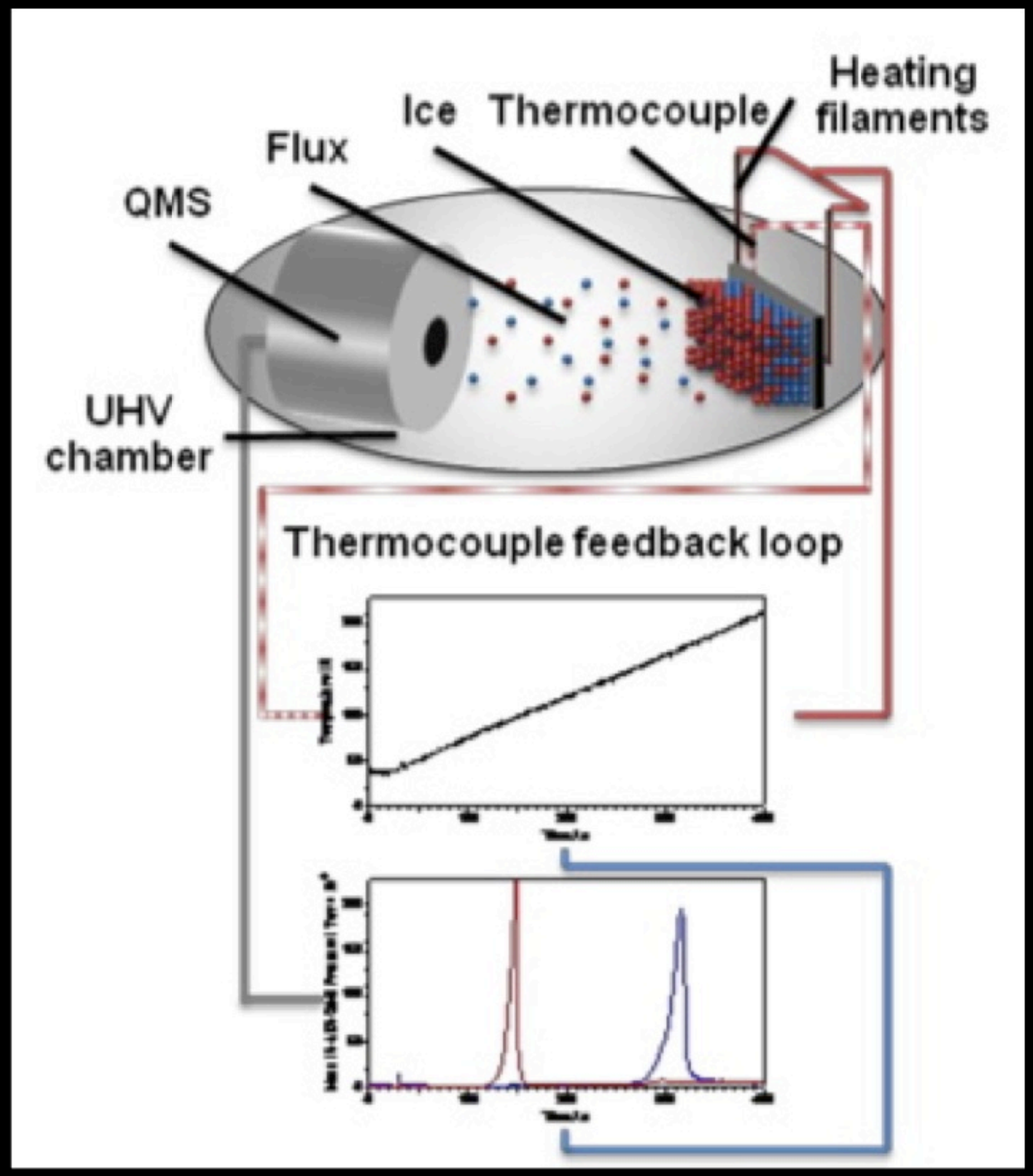


Ultra high vacuum chamber:

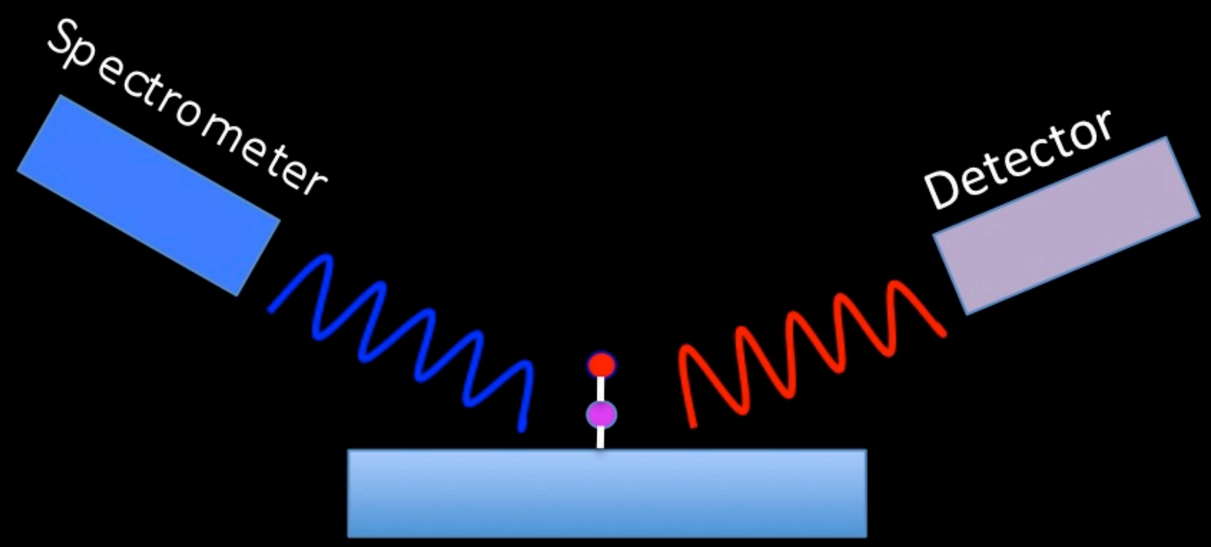
- Base pressure: ≈10^{-10} mbar
- Temperature sample: ≈ 20 K

Experimental techniques

TPD



RAIRS



Initial results

- Improvement of the base temperature of the sample
- Optimization of the atom source
- TPD, RAIRS study of ethene on HOPG

Future projects

- Experimental studies of desorption and molecular formation of sulfur bearing species
- Study of OCS formation:

$$CO + S \rightarrow OCS$$

$$CO + HS + (H) \rightarrow OCS + (H_2)$$

Training (1)

Meetings & LASSIE training:

•Summer school in Leiden (NL) (Astrochemistry lectures, public outreach, time management)

•IAU Symposium (Toledo, Spain)

•Astrochemistry with ALMA (Bologna, Italy)

•Astrosurf meeting (Edinburgh, UK)

Training (2)

UCL Training:

Experimental physical chemistry course

Weekly group meetings and literature discussion

Supervisor meeting

UCL graduate school courses

Assistance in training and supervision of Master’s student

Secondment

Academic: Leiden University, supervisor Prof. Linnartz (early 2012)

Industrial: Currently in discussion with SPECS

Thank you

Fabrizio Puletti
Email:
f.puletti@ucl.ac.uk

Supervisor:
Dr Wendy Brown
Email:
w.a.brown@ucl.ac.uk

MODELLING

THE GAS-GRAIN INTERACTION

Development of astrochemical models based on laboratory data

With the aim of reproducing the observed abundances of molecules in the InterStellar Medium (ISM)

Angela Occhiogrosso, ESR ao@star.ucl.ac.uk

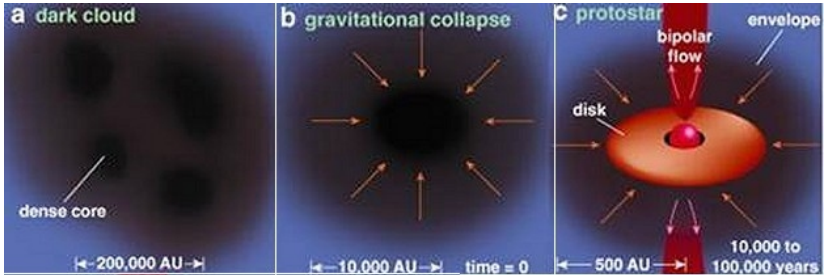
Department of Physics & Astronomy, UCL

Fellowship Start Date: 18/10/2010 - End Date: 17/10/2013

Pricipal Supervisor: S. Viti, Subsidiary Supervisor: W. A. Brown, PI: S. D. Price

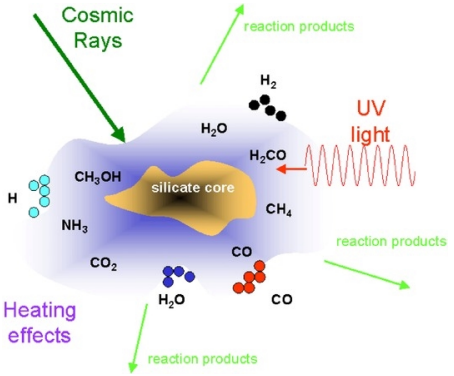
UCL_CHEM chemical model

PHASE I



http://ssc.spitzer.caltech.edu/documents/compendium/galsci

PHASE II



http://www.springerimages.com/Images/Physics

First Results

Monthly Notices of the ROYAL ASTRONOMICAL SOCIETY

Mon. Not. R. Astron. Soc. (2011) doi:10.1111/j.1365-2966.2011.19610.x

A study of methyl formate in astrochemical environments

A. Occhiogrosso,[1]★ S. Viti,[1] P. Modica[2] and M. E. Palumbo[2]

[1]*Department of Physics and Astronomy, UCL, Gower Place, London WC1E 6BT*
[2]*INAF - Osservatorio Astrofisico di Catania, via Santa Sofia 78, 95123 Catania, Italy*

Source	Distance (pc)	Temperature (K)	Observed column density (cm^{-2})	Theoretical column density (cm^{-2})
B1-b dark core	350	<30	8.3×10^{12}	1.2×10^{12}

Work in progress

♦ Electron stimulated desorption of species from H_2O ices. (Secondment's project in collaboration with prof. McCoustra at the Heriot-Watt University)

♦ The chemistry of sulfur-bearing species in the ISM:
- Cosmic ray interactions (Collaboration with dr. M. E. Palumbo, INAF, Catania, Italy);
- Temperature programmed Desorption (TPD)(Collaboration with dr. W. A. Brown, UCL, London, UK);
- Formation, proprierties and reactivity of products (Collaboration with prof. S. Price, UCL, London, UK).

Meeting attended

Annual astrochemical Meeting (Eindhoven, NE)

Summer school (Astrochemistry lectures, Time & management, Outreach activities) (Leiden, NE)

IAU Symposium (Toledo, SP)

Astrochemistry with Alma (Bologna, IT)

Astrosurf Meeting (Edinburgh, UK)

Workshop: 'Challenges in Modelling the Reaction Chemistry of Interstellar Dust' (Leiden, NE).

RAS meetings

My training at UCL

PhD Lectures
Fortran95
Interstellar physics lecture
External & Departmental seminars
SFACE
Group meeting
One to one weekly meeting with my supervisor
Advanced Grammar English
Pronunciation & Public Speaking

Secondment projects

Academic Secondment under the supervision of prof. McCoustra at the Heriot-Watt University (Edinburgh_August 2011)

Future training

♦Industrial Secondment in collaboration with HITEC2000 (Catania, Italy) (January-February)

♦ LASSIE's meetings


Thanks for your attention!

ESR : BINUKUMAR.G.NAIR

SUPERVISOR : Prof. NIGEL J MASON

PROJECT TITLE:SPECTROSCOPY AND CHEMICAL SYNTHESIS OF INTERSTTELLAR ICE ANALOGUES (EXPERIMENTAL STUDY)

AFFILIATION :THE OPEN UNIVERSITY, UK

START DATE :18 OCTOBER 2010

SPECTROSCOPY AND CHEMICAL SYNTHESIS OF INTERSTELLAR ICE ANALOGUES

COMPOSITION

- SIMPLE AND HOMOGENEOUS HYDRO CARBON ICES
- COMPLEX HYDRO CARBONS AND HETROGENEOUS ICES
- SIMPLE AND HOMOGENEOUS HYDRO CARBON ICES ON SILICATE AND CARBON NANO PARTICLES

METHODS

- VUV SPECTROSCOPY
- ELECTRON IRRADIATON
- TPD
- ION IRRADIATION

This project aims to probe the molecular chemistry of interstellar ices under laboratory conditions. Spectroscopic investigation of ices at cryogenic conditions reveals the influence of low temperature chemistry in the formation of complex molecules from simple atoms and radicals. Mimicking the ambient interstellar conditions in the laboratory and monitoring the energetic processing of interstellar ice analogues provides an insight into chemistry of the Universe.

RESULTS

- Prepared an article based on VUV absorption cross-section measurements results of CO_2, C_6H_6, ,$C_2H_4O_2$,HCOOH and $HCONH_2$ ice films(to be submitted).
- Co-authored an article 'Infrared Spectrum of formamide in the Solid Phase' (to be submitted)
- Collected high quality data and contributed to OU Atomic and Molecular Data Centre(VAMDC)
- Posters presented in various conferences and symposium

FUTURE PLANS

- Electron irradiation, VUV spectroscopy and TPD studies of Esters and Alcohols found in interstellar medium.
- Electron, photon and ion irradiation studies of ice films of abundant molecules in ISM, using nano-silicate and nano-carbon dust coated substrate.
- Electron scattering calculations using '*Quantemol*'

CONFERENCES, SUMMER SCHOOLS AND TRAINING EVENTS

1. 4th February 2011 – Belfast, UK – Met with Queen's University LASSIE group, discussed about experiment using ECR source
2. 22nd to 25th February 2011, Presented a poster in Symposium on Atomic, molecular and Optical physics, organized by dept. of Atomic energy, India
3. 10th to 21st March 2011 – Aarhus, Denmark – VUV, Laboratory project –Beam line UV1
4. 17th to 26th May2011–Leiden, Netherlands – Astrochemistry Lecture and LASSIE professional training events.
5. 30th May to 3rd June 2011 – Toledo Spain – IAU conference 'The Molecular Universe'
6. 13th to 17th June 2011 – Bologna, Italy–International Summer School 'Astrochemistry with ALMA'
7. 31st August to 02nd September, 2011'Astrosurf', Heriot Watt University, Edinburgh, UK
8. 12th to 14th October 2011 – Valletta, Malta – COST Conference 'The Chemical Cosmos'

Queens University Belfast

Physical and chemical evolution in Protoplanetary disks

LASSIE MTRM Observatoire de Paris 14th November 2011

Alan McLoughlin

Queen's University Belfast

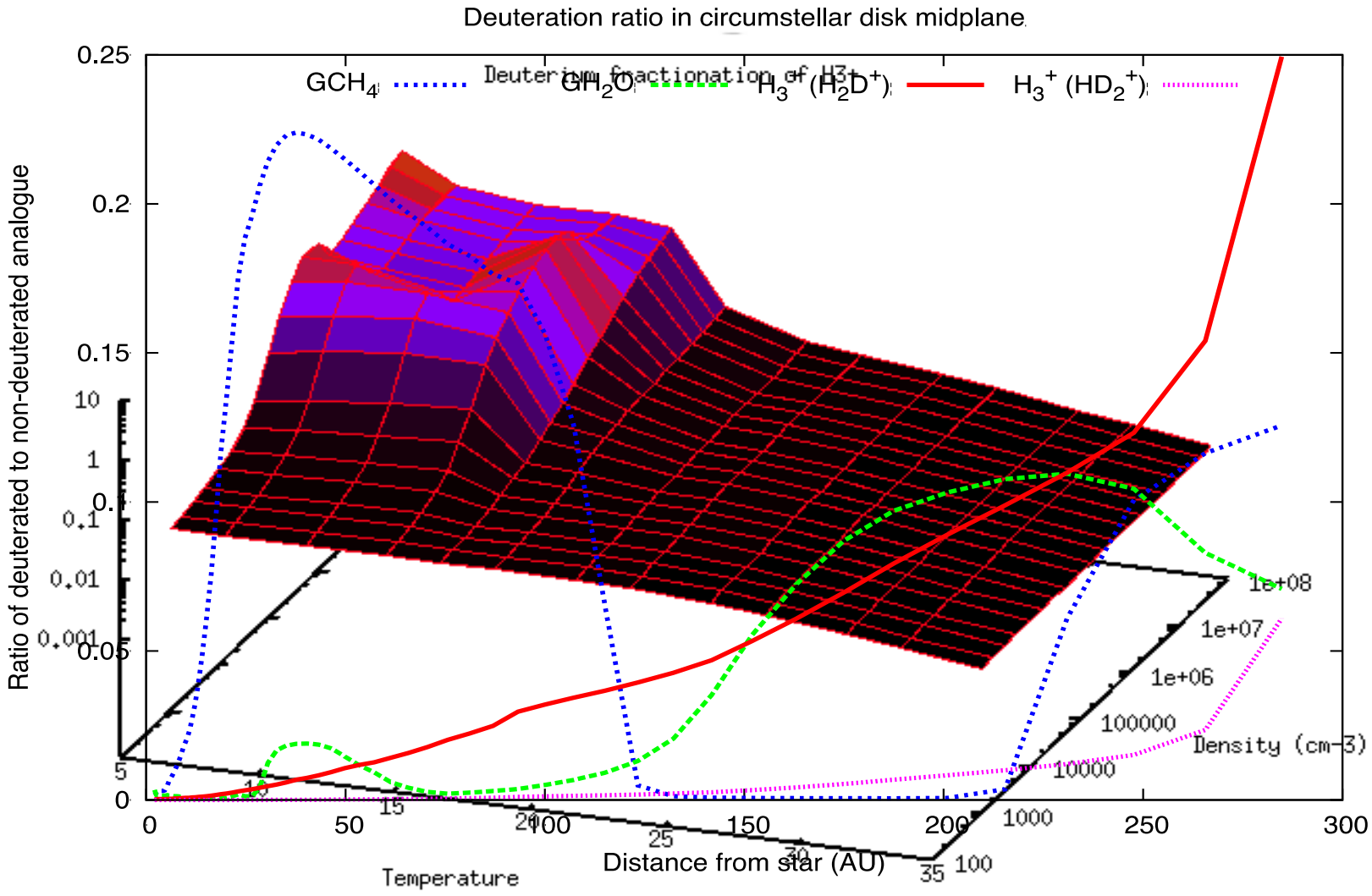
01/10/2010-30/09/2013

Protoplanetary disks

- The project is modelling chemical and physical evolution of protoplanetary disks.
- Using results from LASSIE experimental and theoretical researchers to improve model:
  - Accretion of material onto grains
  - Reactions on the grain surface and within the ice mantle
  - Desorption of material
- Better handling of grain reactions, using modified rate methods to allow use of the modified Arrhenius equation.

Foundational work

- Verified the functioning of basic dark cloud simulation (agreement with theoretical expectation).
- Addition of grain reactions to basic reaction set and adoption of modified rate methods.


Deuteration ratio in circumstellar disk midplane
Deuterium fractionation of H3+
GCH4
GH2O
H3+ (H2D+)
H3+ (HD2+)
Ratio of deuterated to non-deuterated analogue
0.25
0.2
0.15
0.1
0.05
0
10
1
0.1
0.01
0.001
5
10
15
20
25
30
35
0
50
100
150
200
250
300
Temperature
Distance from star (AU)
1e+08
1e+07
1e+06
100000
10000
1000
100
Density (cm-3)

Future work

- Addition of H_2 spin isomers.
- Adopting better grain surface rate calculations.
- Addition of multiply deuterated species.
- Inclusion of new surface chemistry data from the LASSIE network.
- Prediction of observational data and production of simulated ALMA maps.

Training

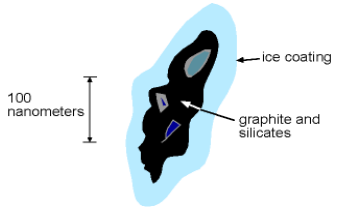
- LASSIE courses:
  - Astrochemistry summer school
  - Astrochemistry with ALMA
- FORTRAN – Armagh Observatory
- ISM lecture course – QUB
- In-house training in chemical modelling
- Attendance at NASA Laboratory Astrophysics Workshop and IAU symposium 280

Laboratory Investigation of Ion Induced Astrochemical Processes on Ices

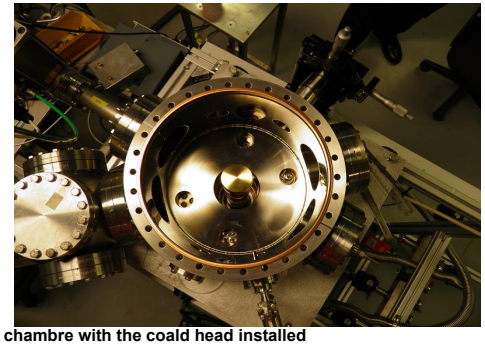
Elena-Andra Muntean , Tom Field and Bob McCullough

Motivation

- the most dominant ice species through the universe is thought to be water ice;
- dust grains are a very important component of the InterStellar Medium and It is believed that many complex molecules are formed on these grains;



A typical dust grain (note the tiny scale!).



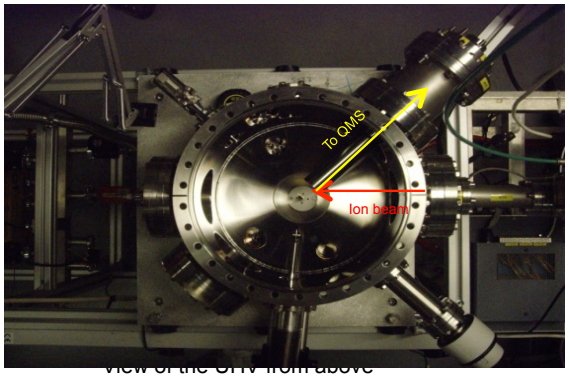
Top view of the UHV chambre with the coald head installed

Experiment and QUB Apparatus

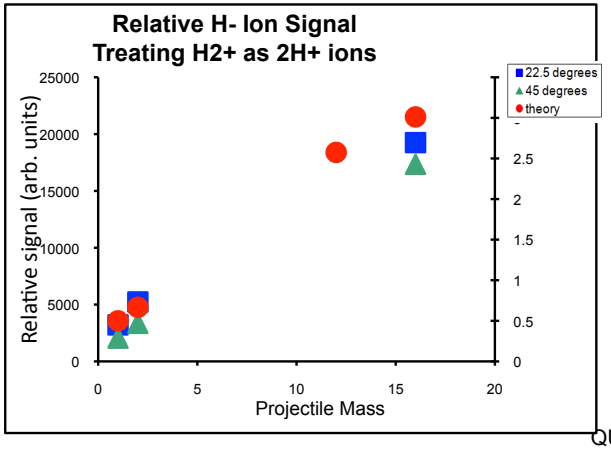
- the experimental set up consists of an ECR ion source, an ion accelerator, a UHV target chamber and QMS for analysis;
- ionic and neutral fragments ejected from the surface during irradiation can be observed with the mass spectrometer, which can detect negative ions, positive ions and neutrals;
- the mass spectrometer will also be used in TPD studies, where the ice sample is warmed up after irradiation and molecules species from the ice are observed;

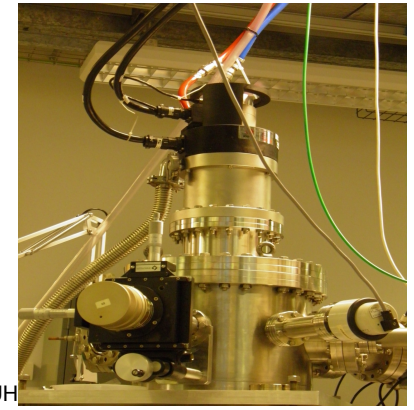
Preliminary experiment

- prior to installation with the cold finger, experiments have been performed to investigate ion irradiation of a titanium surface. In a dissociative electron attachment experiment at the Open University unusual H^- signals were observed, probably from H_2^+ collisions with surfaces giving H^-.
- beams of H_2^+ , D_2^+ , C^+ and O^+ from a 10 Ghz permanent magnet ECR ion source were directed onto a Ti surface at 22.5 deg and 45 deg with respect to the normal of the target surface;
- negative ions from the suraface were directed into the quadrupole by applying a negative bias of 27V to the target;
- H^- ions were observed in this experiment, but they were produced by sputtering and not formed directly from atoms in the primary ion beam;
- below the results obtained are shown with theoretical sputtering intensities; they fit theory well;



View of the UHV from above





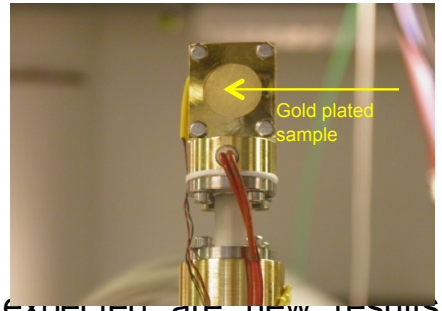
Training , conferences, workshop, courses

- I am very happy that LASSIE gives me the opportunity to participate in workshops, conferences and courses;
- I have taken courses in communicating science through public understanding of science programmes
- I represented LASSIE in public events in Edinburgh, Scotland, and Brussels, Belgium;
- I attended in November 2010 LASSIE & Astrophysical Chemistry Group: Young Researchers Meeting;
- thanks to LASSIE I attended the International Summer School in Bologna about the new facility ALMA and the courses about astrochemistry held in Leiden;
- in Leiden I also attended the additional training about time and project management;
- in October 2011 I participated at the Annual Conference-The Chemical Cosmos;
- I attended an Atomic and Molecular Physics course from QUB and I passed the exam;
- the post-graduate training support unit in Belfast runs a variety of courses and I participated to some of them and I will participate in the future in order to improve my communication skills;
- conferences are excellent networking opportunities as are workshops. The upcoming conferences and workshops of LASSIE and outside the network described will be good opportunities for me to attend them – and also the work placements (the industrial partners and other universities);
- I have received and I will continue to receive training from my supervisors in using the vacuum equipment, running the ECR ion source and mass spectrometry;

Work in progress and future work

- a new experimental apparatus is being developed to investigate interactions of singly and multiply charged ions with analogues of astrophysical ice;
- we have recently installed the cold head, which can go down to ~ 10 K or lower, with a sample holder into the UHV chamber;
- we are developing the experimental set-up and run different test to make sure everything works fine;
- all the pieces from the experiment starting with the UHV chamber are new for this project and also the controllers and units have to be special made for this experiment;

The temperature controlled sample holder on cold-head



Expectations

- the major accomplishments that are expected are new results in the area of irradiation of astrophysical ice analogue. In particular, the capability to generate high currents of multiply charged ions, such as C^{2+}, C^{3+}, O^{2+} etc. is unique to this experiment in Belfast;
- more broadly, it is expected that the results will give more insight into the formation of molecules on astrophysical ices in the interstellar medium;
- disseminate results in LASSIE and more widely for inclusion in astrochemical models

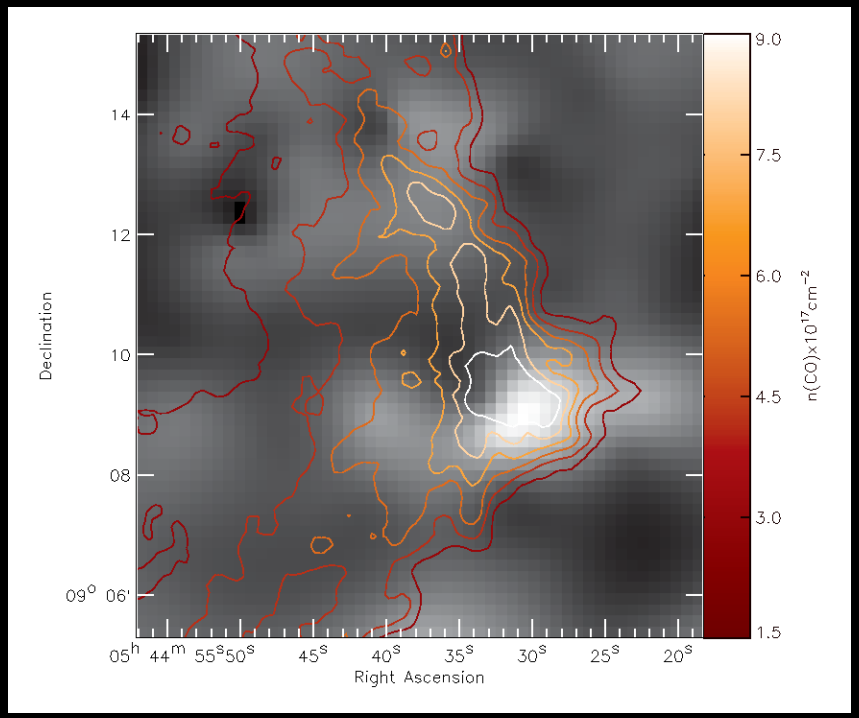
Acknowledegement: This project work is fully funded by LASSIE FP7 Marie Curie Initial Training Network (ITN).

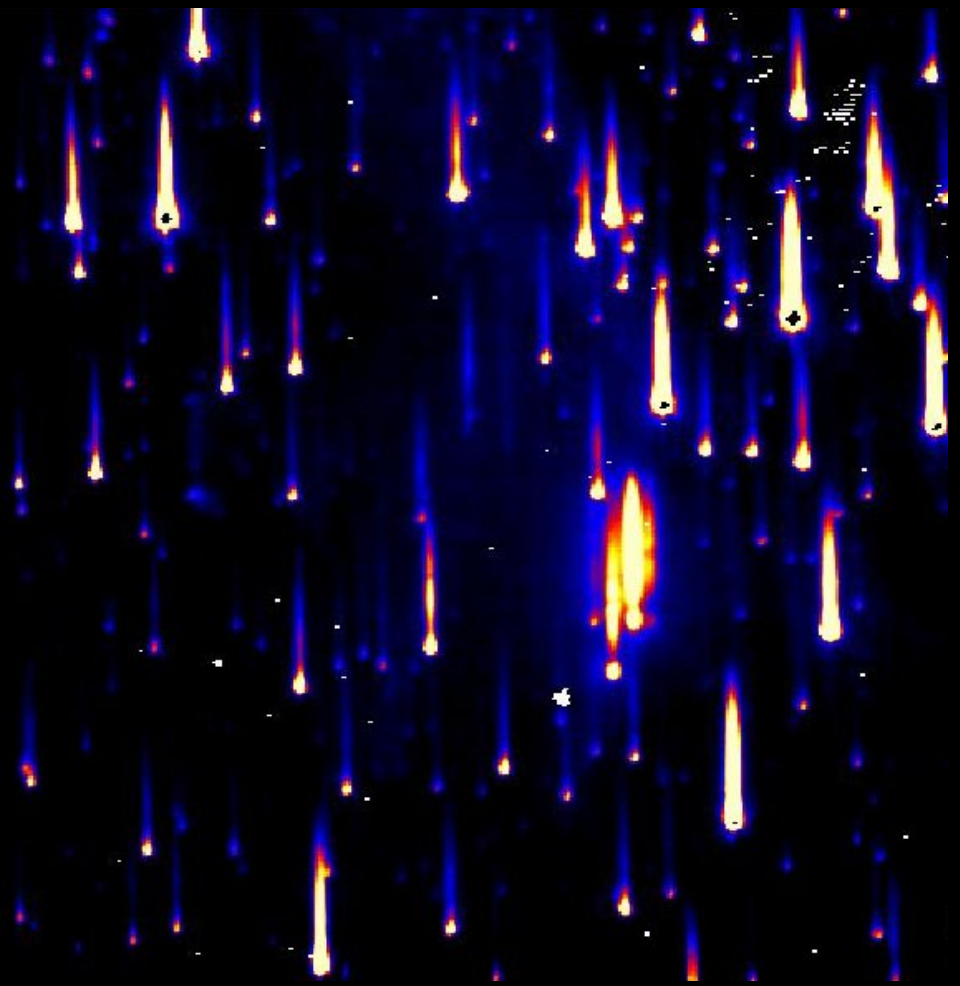
Combined Gas-Ice Mapping of 1000 AU Scales of Star Forming and Pre-Stellar Cores

University of Strathclyde Glasgow

A.N. Suutarinen H.J. Fraser J.A. Noble

Our objective: To do ice mapping in cold cloud cores to test our current understanding of related chemistry. (*Theme 5*)





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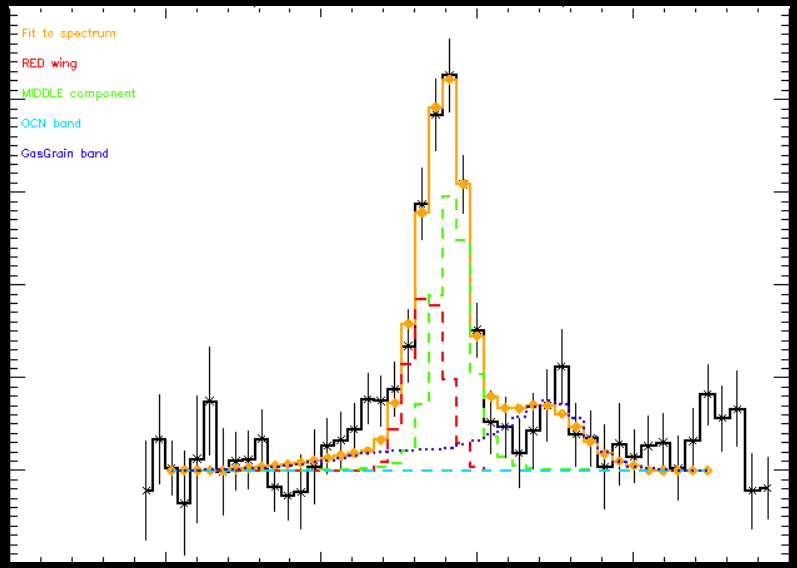
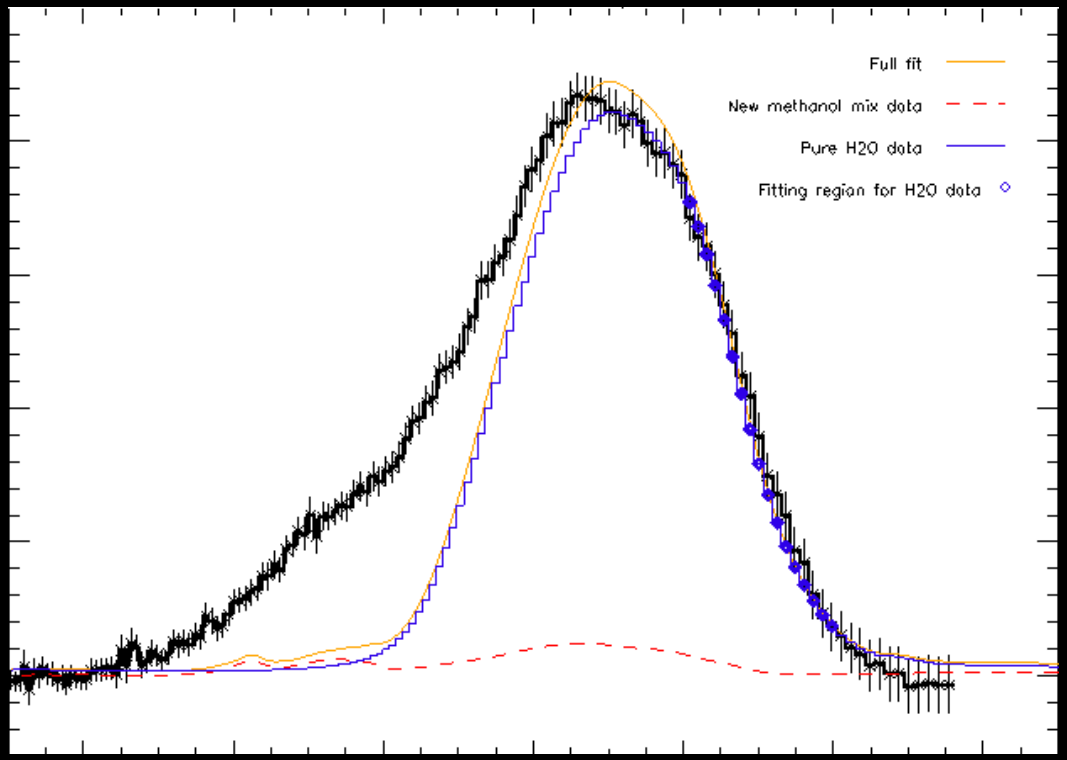
Work with other LASSIE groups: *Isokoski & Linnzartz* - combining our AKARI data with their lab data.





Future work planned with:

M.E. Palumbo (Catania) - CO_2 fitting accounting for experimental results from LASSIE showing C-grain production of CO_2 to account for breadth of observed feature

Ant Jones (Paris) - C-H fitting in 3.4 micron region - account for the real effects of grain surface hydrogenation

Combined Gas-Ice Mapping of 1000 AU Scales of Star Forming and Pre-Stellar Cores

University of Strathclyde Glasgow

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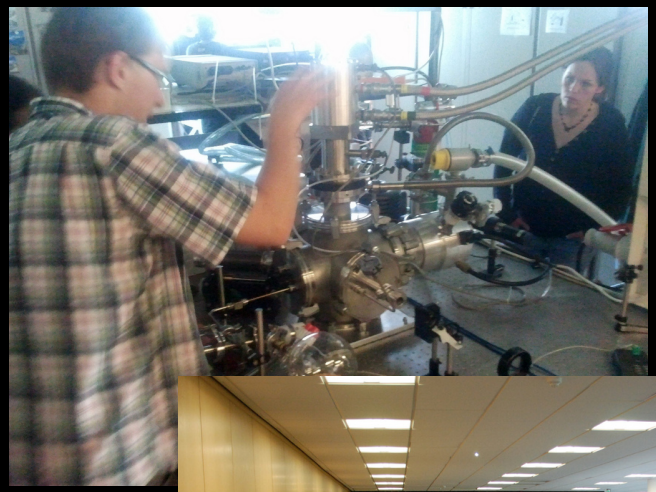

LASSIE - Because good science needs good people

Predicting the structure of amorphous solid water

Pavel D. Elkind

Strathclyde University
Glasgow, Scotland, UK

LASSIE
Theme 4

Paris
14-11-2011

Objectives

- Predict at the molecular level the structure of interstellar water and water-CO ices
- Investigate the photochemical routes of formation of new molecules on these ices
- Improve the existing astrochemical models by providing new reaction rates

Objectives

- Predict at the molecular level the structure of interstellar water and water-CO ices
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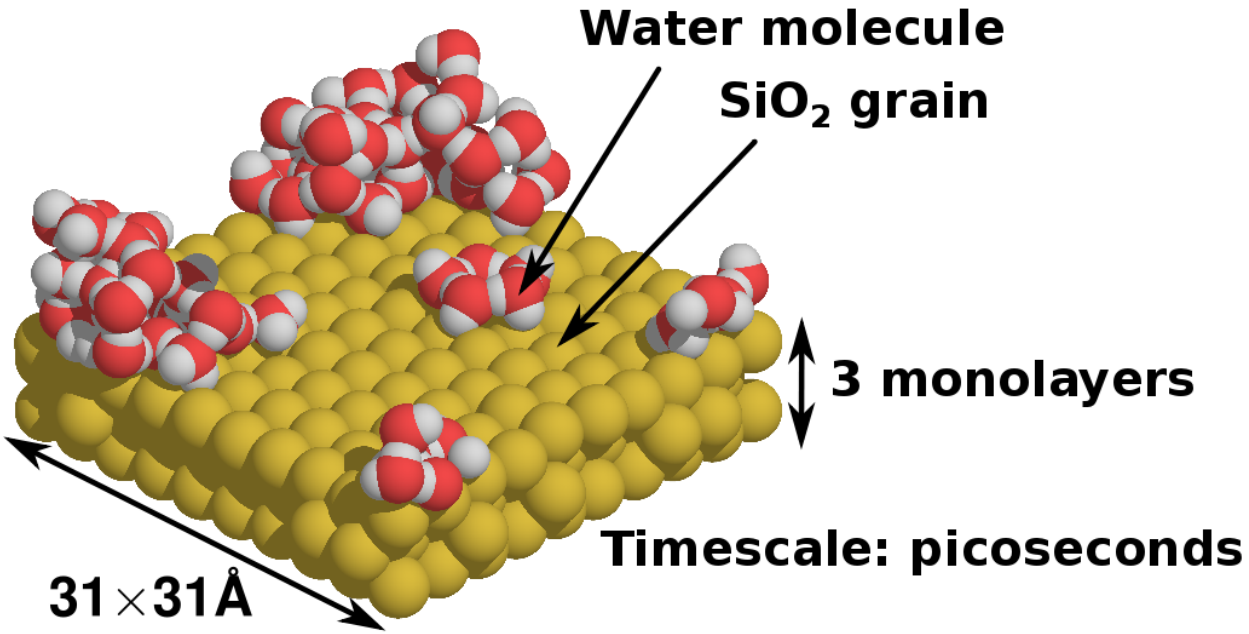
- Improve the existing astrochemical models by providing new reaction rates

Methodology: Classical Molecular Dynamics



One-by-one “deposition” of water molecules (TIP4P potential) on the coarse-grained silica surface (Lennard–Jones potential).

<Movie>

Results

- Amorphous water ices have tower-like structure and are highly porous
- Porosity shows little dependence on the substrate temperature

Results

- Amorphous water ices have tower-like structure and are highly porous
- Porosity shows little dependence on the substrate temperature

LASSIE:

- Ice structures are the deliverables

Collaborations

LASSIE

- University of Göteborg, Sweden – academic placement, with Prof. Gunnar Nyman and Dr. Stefan Andersson
- Leiden University, Netherlands – CO-CO potential, with Prof. Mark van Hemert and Prof. Ewine van Dishoek
- Leiden University, Netherlands – experimental study of ice porosity, with Karoliina Isokoski and Prof. Harold Linnartz

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Non-LASSIE

- The University of Iceland – Adaptive Kinetic Monte–Carlo approach, with Dr. Andreas Pedersen
- The Radboud University, Netherlands – ice structures, with Leendertjan Karssemeijer and Dr. Herma Coupen
- The University of Innsbruck, Austria – neutron scattering study of ice structure, with Prof. Thomas Lörting

Thank you!