

LASSIE-ITN
Mid-Term Review Meeting
14th November 2011



Venue: Observatoire de Paris, Salle du Conseil

Agenda

Morning meetings: 10:00 – 12:30;

Afternoon meetings: 13:30 – 16:30

10:00 Welcome – Dr. Claude Catala, President of the Observatoire de Paris

10:00-10:40 Coordinators' Reports

1. Overview – Prof Martin McCoustra
2. Training Coordination Group – Dr Lijv Hornekær
3. Research Coordination Group – Prof Harold Linnartz
4. Outreach & Promotion Group – Prof Nigel Mason

10:40-11:10 PI Reports

A short report from a representative of each beneficiary.

11:10-11:20 Coffee Break

11:20-12:30 Fellows Reports

- (1) John Thrower, (2) Farahjabeen Islam, (3) Divya Sharma,
(4) Demian Marchione, (5) Andrew Cassidy, (6) Lisseth Gavilan,
(7) Ischraf Oueslati, (8) Rachid Tchala, (9) Guillem Aumatell-Gomez,
(10) Tushar Suhasaria, (11) Tolou Sabri, (12) Tobias Albertsson, (13) Siyi Feng

12:30-13:30 Lunch Break

13:30-15:00 Fellows Reports Continued

- (14) Steven Cuyllé, (15) Gleb Fedoseev, (16) Irene San Jose Garcia,
(17) Anna Clemens, (18) Bethmini Senevirathne, (19) Fabrizio Puletti,
(20) Angela Occhiogrosso, (21) Ewelina Szymanska, (22) Binukumar Nair, (23) Alan
McLoughlin, (24) Elena-Andra Muntean, (25) Aleksu Suutarinen, (26) Pavel Elkind

15:00-16:00 Face-to-face meetings with Research Fellows

A meeting between the Project Officer and Expert External Reviewer and the ESRs
and ERs

16:00-16:30 Wrap-up Meeting

A meeting between the Project Officer and Expert External Reviewer and the REA-
PIs

15:45-16:15 Coffee Available



LASSIE FP7 ITN LABORATORY ASTROCHEMICAL SURFACE SCIENCE IN EUROPE

Grant Agreement 238258

SEVENTH FRAMEWORK PROGRAMME INITIAL TRAINING NETWORKS



2011 Young Astronomers' Meeting (YAM)
November 15th 2011, Paris, France

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OVERVIEW
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PUBLICATIONS
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The European Commission has recently approved under the Framework 7 Programme the ITN-People network LASSIE; a large interdisciplinary training network in the field of SOLID STATE ASTROCHEMISTRY established with the goal of addressing issues of relevance to the chemical evolution of the Universe. From 01/02/2010 and over the next 4 years, a consortium of 13 experimental and theoretical groups with 5 industrial and 1 outreach partners, led by Professor Martin McCoustra (Heriot-Watt University, Edinburgh, UK), will supply training and research opportunities for up to 28 Early Stage Researchers (ESR, PhD students) and 4 Experienced Researchers (ER, Post-doctoral research assistants) at the following host sites:

Prof. M.R.S. McCoustra	Heriot-Watt University, Edinburgh, UK
Dr. L. Hornekaer	Aarhus University, Denmark
Prof. J. L. Lemaire	Paris Observatory, France
Prof. H. Zacharias	University of Münster, Germany
Dr. C. Jäger	Max Plank Gesellschaft, Germany
Dr. M. E. Pulumbo	National Institute for Astrophysics, Catania, Italy
Prof. H. Linnartz	Leiden University, Netherlands
Prof. D. Chakarov	Chalmers University, Gothenburg, Sweden
Prof. G. Nyman	University of Gothenburg, Sweden
Prof. S. D. Price	University College London, UK
Prof. N. J. Mason	The Open University, UK
Dr. T. A. Field	Queen's University, Belfast, UK
Dr. H. J. Fraser	Strathclyde University, Glasgow, UK

5746 visits

To qualify as an Early Stage Researcher (ESR), candidates must have obtained a Masters Degree or equivalent in Chemistry, Physics, Astronomy or a related Engineering field within the past four years and demonstrate experience in experimental physics, chemical physics, physical chemistry, surface science, computational chemistry and astronomy, or theoretical astrochemistry and astrophysics. Applicants considering themselves as Experienced Researchers (ER) must already possess a Doctoral Degree or have at least 4 years of research experience (full time equivalent) since obtaining their Masters Degree. They must also have relevant expertise in



LASSIE FP7 ITN

LABORATORY ASTROCHEMICAL SURFACE SCIENCE IN EUROPE

SEVENTH FRAMEWORK PROGRAMME INITIAL TRAINING NETWORKS



Appointed people

Beneficiary Name	ER Name [P=poster]	ESR Name(s) [P=poster] [supervisor] 01/02/2010	ESR Name(s) [P=poster] [supervisor] 01/02/2011
Heriot-Watt University	pending [P]	pending [P] [Martin McCoustra]	Divya Sharma [P] - Demian Marchione [P] [M.J Paterson & M.R.S McCoustra] - [M.R.S McCoustra]
Aarhus University	John Thrower [P]	Andrew Cassidy [P] [Liv Hornekaer]	vacant [P] [supervisor]
Paris Observatory		Lisbeth Gavilan [P] [Jean Louis Lemaire]	Ichraf Oueslati [P] - Rachid Tchalala [P] - pending [P] [N. Feautrier] - [H. Oughaddou] - [supervisor] [B. Kerkeni] - [JL. Lemaire] - [supervisor]
University of Münster		Guillem Amatell Gomez [P] [Gerhard Wurm]	Tushar Suhasaria [P] [H. Zacharias]
Max-Planck-Gesellschaft		Tolou Sabri [P] - Tobias Albertsson [P] [Cornelia Jager] - [Thomas Henning]	Sivi Feng [P] [Henrik Beuther]
National Institute for Astrophysics	Farahjabeen Islam [P]		
Leiden University		Steve Cuytle [P] - Gleb Fedoseev [P] [Harold Linnartz] - [Harold Linnartz]	Irene San José Garcia [P] - Agata Karska [P] [Ewine van Dishoeck] - [Ewine van Dishoeck]
Chalmers University		Anna Clemens [P] [Dinko Chakarov]	vacant [P] [supervisor]
University of Gothenburg	Dylan Drake-Wilhelm [P]	Pulasthika B. Senevirathne [P] [Gunnar Nyman]	Pavel Elkind [P] [G. Nyman & H. J. Fraser]
University College London		Fabrizio Puletti [P] [Wendy Brown]	Angela Occhiogrosso [P] [Serena Viti]
The Open University		Ewelina Szymanska [P] [Nigel J Mason]	Binukumar G Nair [P] [Nigel J. Mason]
Queen's University, Belfast		Elena-Andra Muntean [P] [Tom Field]	Alan McLoughlin [P] [Tom Millar]
Strathclyde University		Pavel Elkind [P] [H. J. Fraser & G. Nyman]	Aleksi Suutarinen [P] [H. Fraser]

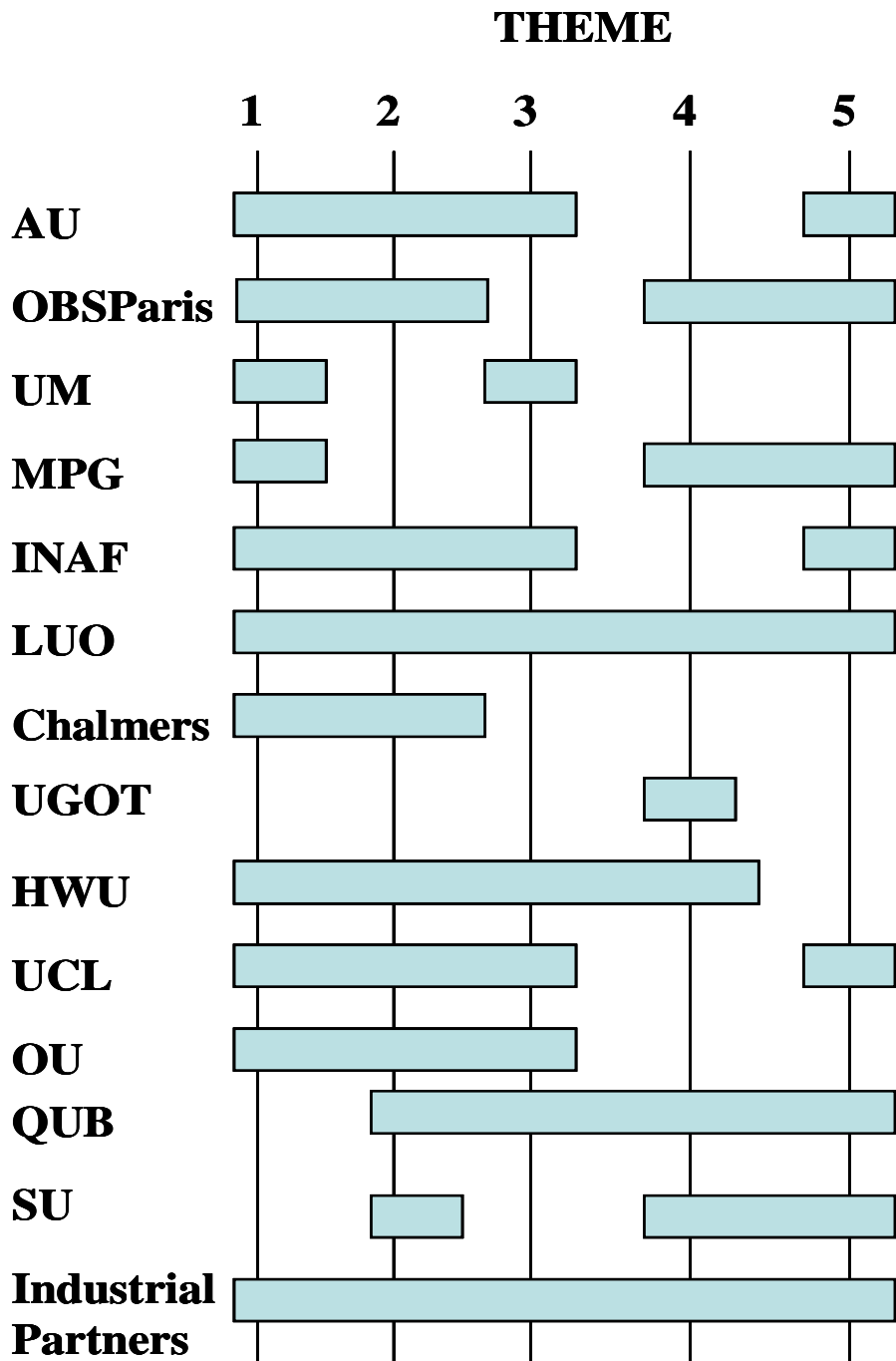
Theme 1 - Formation of Grains, Small Molecules and Ices

Theme 2 - Physical Processes in and on Icy Grains

Theme 3 - Chemical Transformations in and on Icy Grains

Theme 4 - Modelling the Gas-Grain Interaction

Theme 5 - Observations and Astronomical Models Involving Dust and Ices



Heriot-Watt University



Heriot-Watt University (HWU) contributes to research in role in Work Packages 1, 2, 3 and 4.

WP 1: Formation of grains, small molecules and ices.

- Formation of water via reactions of H and O atoms on silica surfaces:
 - rates and mechanisms.
 - morphology of water ice.
 - spectroscopy of water ice product.

WP 2: Physical processes in and on icy grains

- Thermal desorption of ices.
- Electron induced desorption of ices.
- Photon induced desorption of ices.
- Morphology changes in ices due to thermal, electron and photon induced processing.

WP 3: Chemical transformation in and on icy grains.

- Electron induced chemistry in ices.
- Photon induced chemistry in ices.
- Chemistry induced by atomic and radical bombardment.

WP 4: Modelling that gas-grain interactions.

- Computational modelling of the dynamics of photon induced desorption and dissociation.
- Computational calculation of IR and UV spectra of ices.



👉 Academics

- Professor Martin McCoustra
 - Chair in Chemical Physics
- Dr Martin Paterson
 - Lecturer. Theoretical and Computational Chemistry

www.astrochemistry.hw.ac.uk

www.che.hw.ac.uk/TMS/

👉 Post Docs

- Dr Mark Collings
 - LASSIE Network Manager
- Dr Jerome Lasne
 - LASSIE ER: Experimental studies (WP 1, 2, 3)

👉 Students

- Divya Sharma
 - LASSIE ESR: Computational studies (WP 4)
- Demian Marchione
 - LASSIE ESR: Experimental studies (WP 2, 3)
- Ali Abdulgalil
 - Final Year PhD Student: experimental studies (WP 2, 3)
- Victoria Frankland
 - PhD Student (now submitted) (WP 1)

Aarhus University

Department for Physics & Astronomy Aarhus University, Denmark AU



Researchers involved

PI's involved:	Assoc. prof. Liv Hornekaer	Prof. David Field
LASSIE ER	John Thrower	
LASSIE ESR		Andrew Cassidy
LASSIE ESR	NN	
Involvement of Non-LASSIE Post. Docs.:	Richard Balog	Oksana Plekan Cecile Favre
PhDs:	Louis Nilsson Mie Andersen	

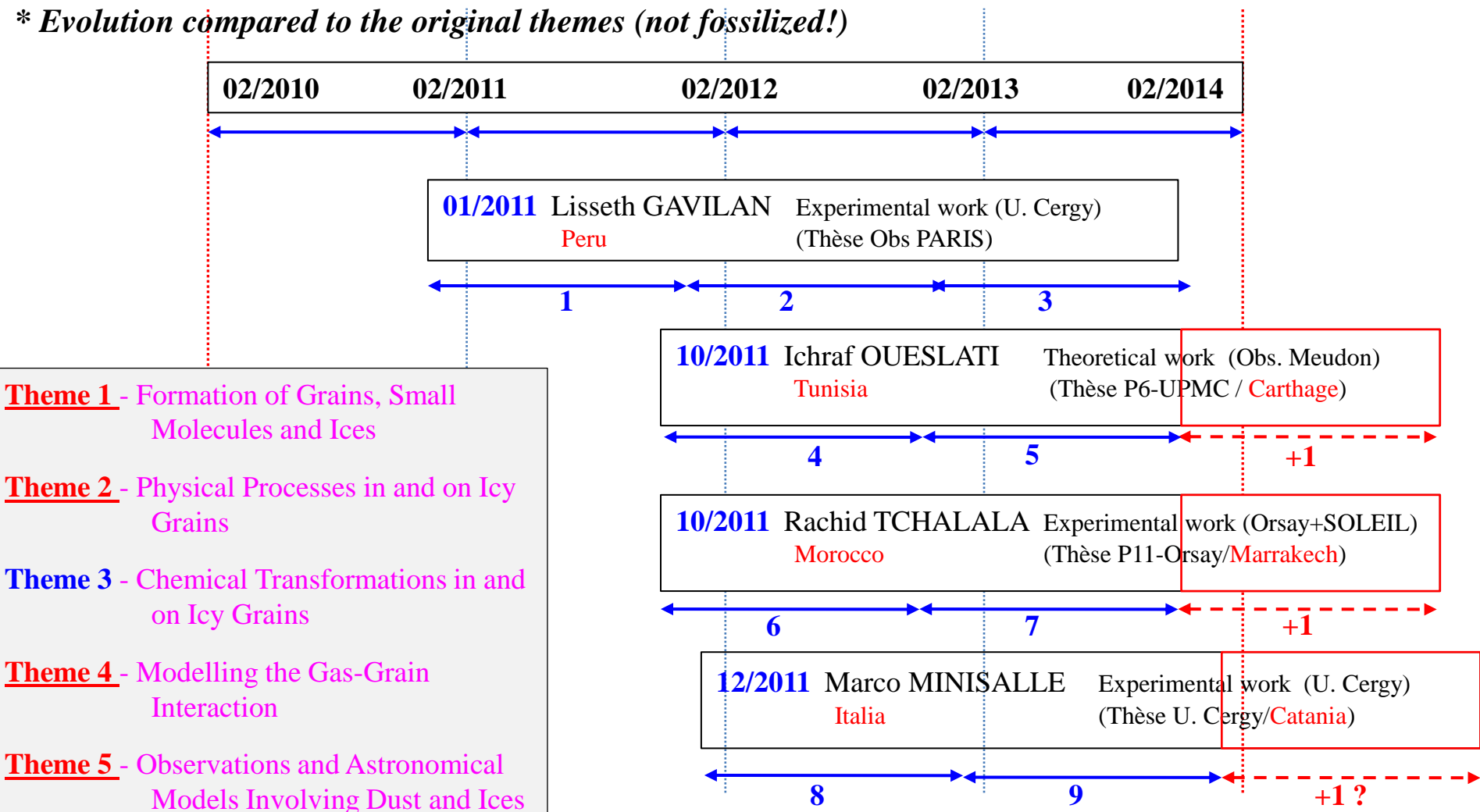
Research Objectives

- 1.03 Small molecule formation on carbon surfaces
 - scanning tunnelling microscopy (STM) and thermal desorption spectroscopy (TPD) [JT, AMC, LH]
- 1.04 Morphology of ices formed reactively on carbonaceous surfaces
 - STM and low energy electrons [AMC, LH, DF]
- 3,01; Construction and optimization of low energy electron source
 - ASTRID storage ring [AMC, DF]
- 3.03 + 3.05 Photon induced chemical transformations in HPAHs
 - TPD, STM [JT, LH]
- 3.04 Investigate low energy electron-induced chemistry within ices [AMC, DF]
- 3.06 Atom induced chemical transformation in PAH films
 - TPD, STM [JT, AMC, LH]
- 4.04 Modelling – understanding H_2 formation on carbonaceous surfaces
 - Density functional theory calculations [LH]

Paris Observatory

** Involvement with several complementary research group in the institution or outside (in particular in the framework of co-tutelles).*

** Evolution compared to the original themes (not fossilized!)*



LASSIE Early Stage Researchers

Liseth GAVILAN (3 years)

Gas-grain interactions in interstellar conditions (laboratory and observational astrophysics)

* *Observatoire de Paris & Université de Cergy-Pontoise*: Prof J.L. **Lemaire**

Collaborations and secondments inside LASSIE: (C. Jäger, Jena, silicates), (D. Field, Aarhus, Observations) and outside: (G. Vidali Syracuse USA, experiments)

Formation of H₂ (and other molecules) on silicates investigated in the laboratory (FORMOLISM experiment: TPD, REMPI/TOF, RAIRS and AFM/STM, PES) under interstellar conditions

Ichraf OUESLATI (2 years)

Theoretical study of molecular hydrogen formation in the ISM

Observatoire de Paris: Dr. **N. Feautrier**, Dr. **A Spielfiedel**

* *Université Paris VI, UPMC*: Prof. **L Tchang-Brillet**

* *Université de Carthage Tunisie*: Prof. **B. Kerkeni**

Formation of H₂ on silicates investigated using DFT and hybrid QM/MD methods

Rachid TCHALALA (2 years)

Experimental study of molecules formation in the ISM

* *Université Paris XI, ORSAY, Laboratoire ISMO*: Prof. **H. Oughaddou**, Dr.. **G. Dujardin**

* *Université de Marrakech*: Prof. **A. Ali**

Collaborations and secondments inside LASSIE : (Prof J.L. Lemaire, experiments) and outside: (Dr. R. Belkhou, Synchrotron SOLEIL and Prof. T. Greber, Zürich, PES)

Interaction and reactivity of hydrogen and oxygen on surfaces simulating interstellar grains (SiC, Graphene, Silicene) in the laboratory (AFM-STM, PES, Synchrotron)

Marco MINISALE (2 years)

Experimental studies of the gas-grain interaction in an astrophysical context

* *Observatoire de Paris & Université de Cergy-Pontoise*: Prof . **F. Dulieu**

* *Università di Catania*: Prof. **V. Pirronello**

Theme 1 - Formation of Grains, Small Molecules and Ices: Formation and optical properties of dust grains, formation of small molecules on grains and the reactive accretion of icy layers and the morphological and spectroscopic properties of the resulting icy films. Provide a basic understanding of grains and ices.

- The release of reaction energy into product translation, rotation and vibration in the heterogeneous formation of small molecules on model dust grain surfaces (AU, Chalmers, INAF, OBSParis, UCL, UM).*
- The rates of molecule and ice formation on dust grain surfaces, including studies of isotopic fractionation (AU, Chalmers, HWU, LUO, INAF, OBSParis, UCL).*
- The morphology of ices formed reactively on model grain surfaces (AU, Chalmers, HWU, INAF, OBSParis, UCL).*
- The infrared, optical and ultraviolet (UV) spectroscopy of ices formed reactively on model dust grain surfaces (Chalmers, HWU, LUO, OU, UCL).*

Theme 2 - Physical Processes in and on Icy Grains: Understanding physical processes occurring when an icy mantle is subjected to EM radiation or bombarded with charged and/or neutral particles

- Thermal desorption of simple ices, complex mixed ices and clathrates as observed in the cold, dense regions of the ISM associated with star formation (Chalmers, HWU, LUO, OBSParis, SU, UCL).*
- Desorption of simple ices, complex mixed ices and clathrates induced through interaction with electromagnetic radiation (Chalmers, HWU, LUO, OU, UCL, SU).*
- Desorption of simple ices, complex mixed ices and clathrates induced via interaction with low energy electrons and models of cosmic rays (Partners AU, Chalmers, HWU, INAF, OU, QUB).*
- Role of heat, electromagnetic radiation and cosmic rays in promoting changes in ice morphology (HWU, LUO, INAF, OU, UCL, SU).*

Theme 3 - Chemical Transformations in and on Icy Grains: Study the evolution and simulate the formation of complex molecules of astrophysical interest on grains and in interstellar ices. [UHV conditions, ice morphology (chemical composition, amorphous/crystalline structure, pure/layered or mixed configurations), ice temperature and thickness. Quantify influence of different chemical trigger mechanisms under conditions typical for inter- and circumstellar matter.

- *UV photon- and low energy electron-induced, VUV, XUV and X-ray photon- and cosmic ray-induced chemical transformations*
- *Chemical transformations following atom, radical or thermal molecular ion*

Theme 4 - Modelling the Gas-Grain Interaction: Computational modeling programme

- *Developing models of amorphous ices and dust grains (OBSParis, LUO, SU, UGOT, QUB).*
- *Understanding the dynamics of photon-driven processes in amorphous ices, including photodesorption and photodissociation (HWU, OBSParis, LUO, UGOT).*
- *Understanding molecular hydrogen formation on graphite and amorphous ice (OBSParis, LUO, UGOT, QUB).*
- *Understanding the hydrogenation reactions of CO in various types of ice, particularly CH₃OH formation (OBSParis, LUO, UGOT, QUB).*
- *Simulating diffusion of hydrogen atoms and oxygen atoms on hexagonal, cubic and amorphous ices (OBSParis, UGOT).*
- *Simulating the condensation and growth of grains (MPG).*
- *Simulating the growth and evolution of water ice and other solids under interstellar conditions (LUO).*

Theme 5 - Observations and Astronomical Models Involving Dust and Ices: Obtain quantitative astronomical constraints on the role of grains in interstellar chemistry. Achieved through a combination of observations and modelling. closely linked with laboratory work.

- *Large and small scale maps of infrared lines of H₂ and deuterated species will be constructed to trace its formation on grain surfaces under different conditions (AU, OBSParis).*

University of Münster

Processes on grains and ices

Gerhard Wurm

Helmut Zacharias

Institute for Planetology and Physics Institute
University of Münster

Wilhelm-Klemm-Str. 10
48149 Münster
Germany

Objectives

Evolution of water-ice in the context of planet formation
(aggregation, sublimation, gas flow)

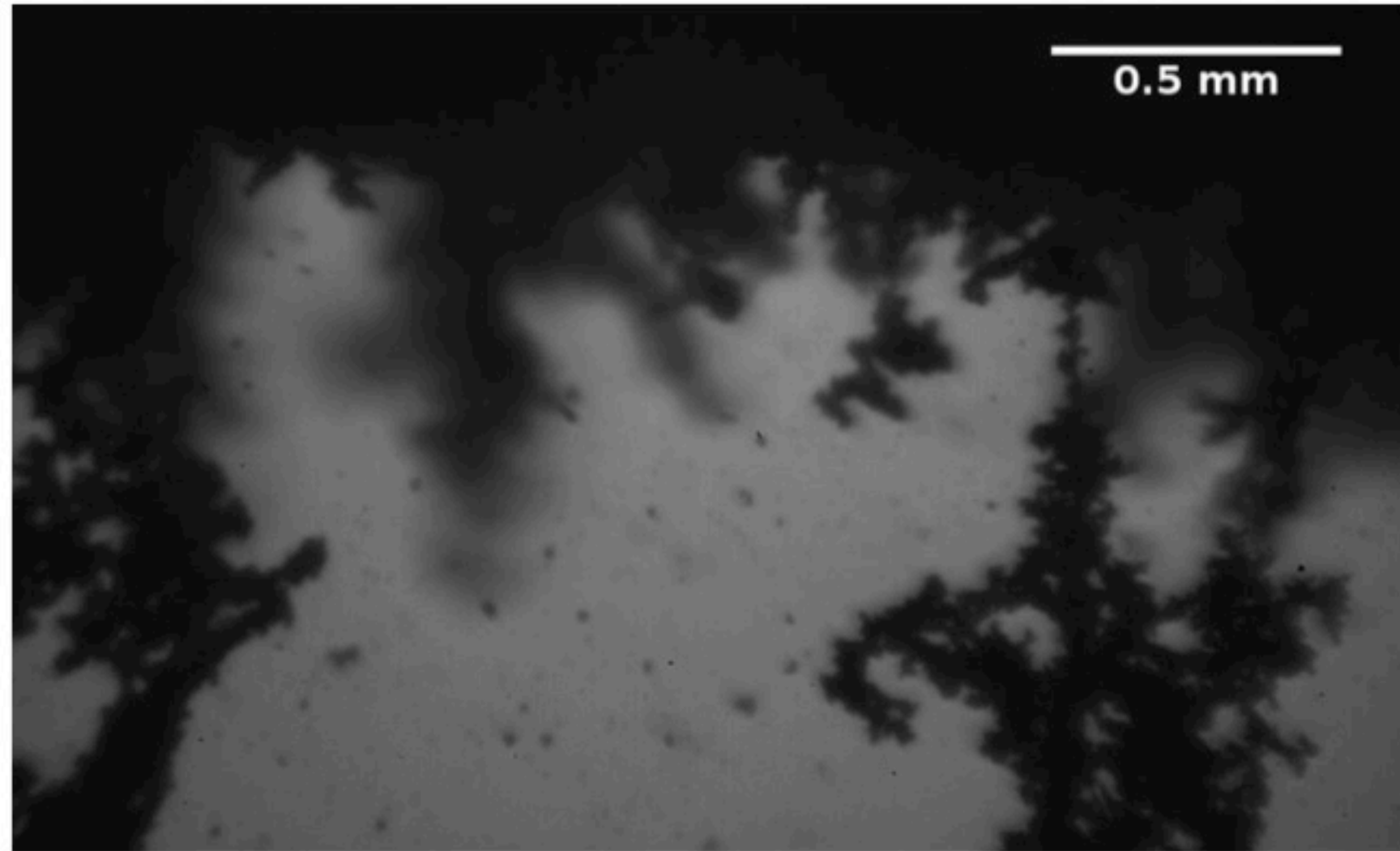
ESR: Guillem Aumatell (Spain), since August 2010

Photochemical processes in doped ices

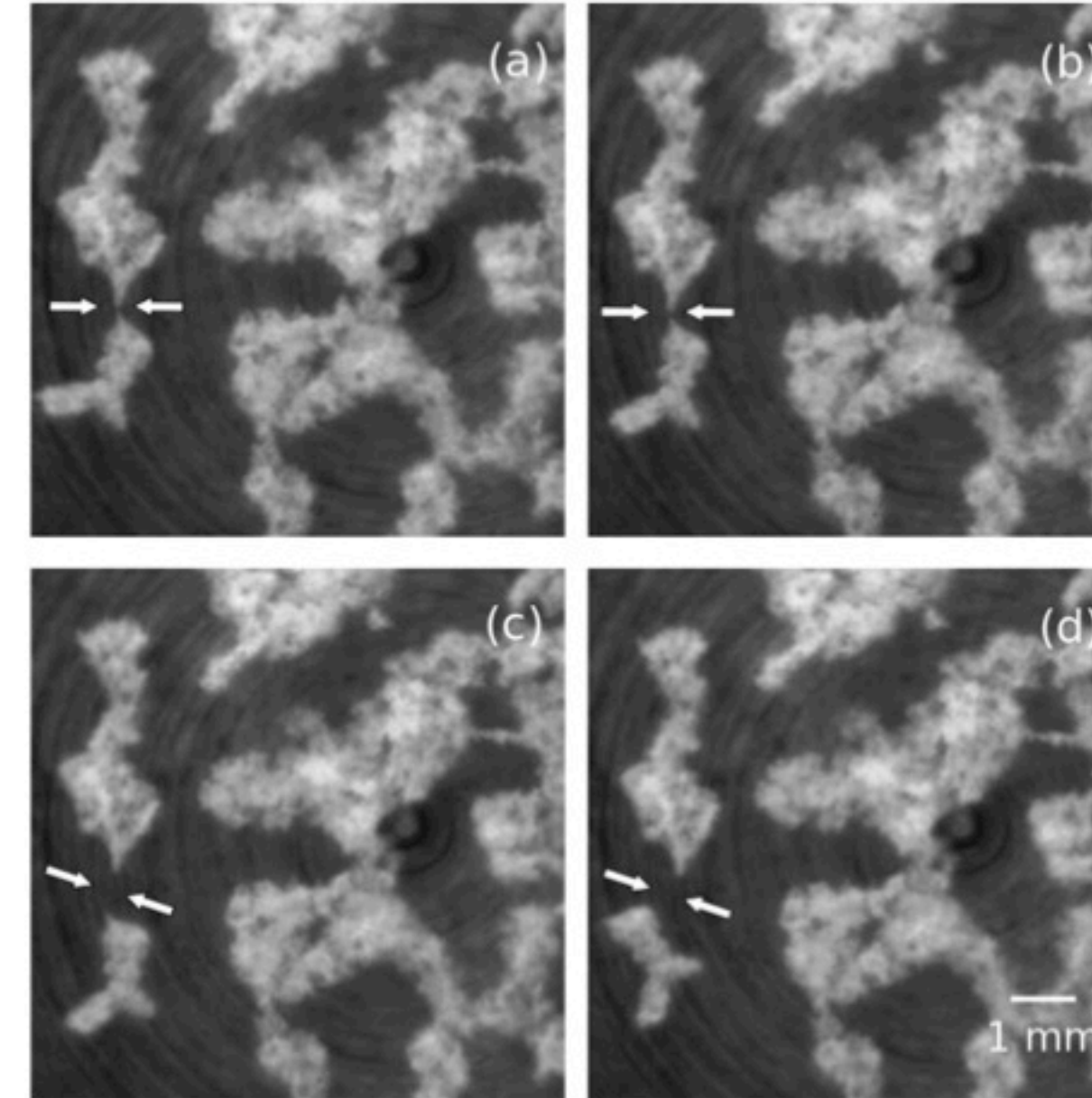
ESR: Tushar Suhasaria (India), since October 2011

Results

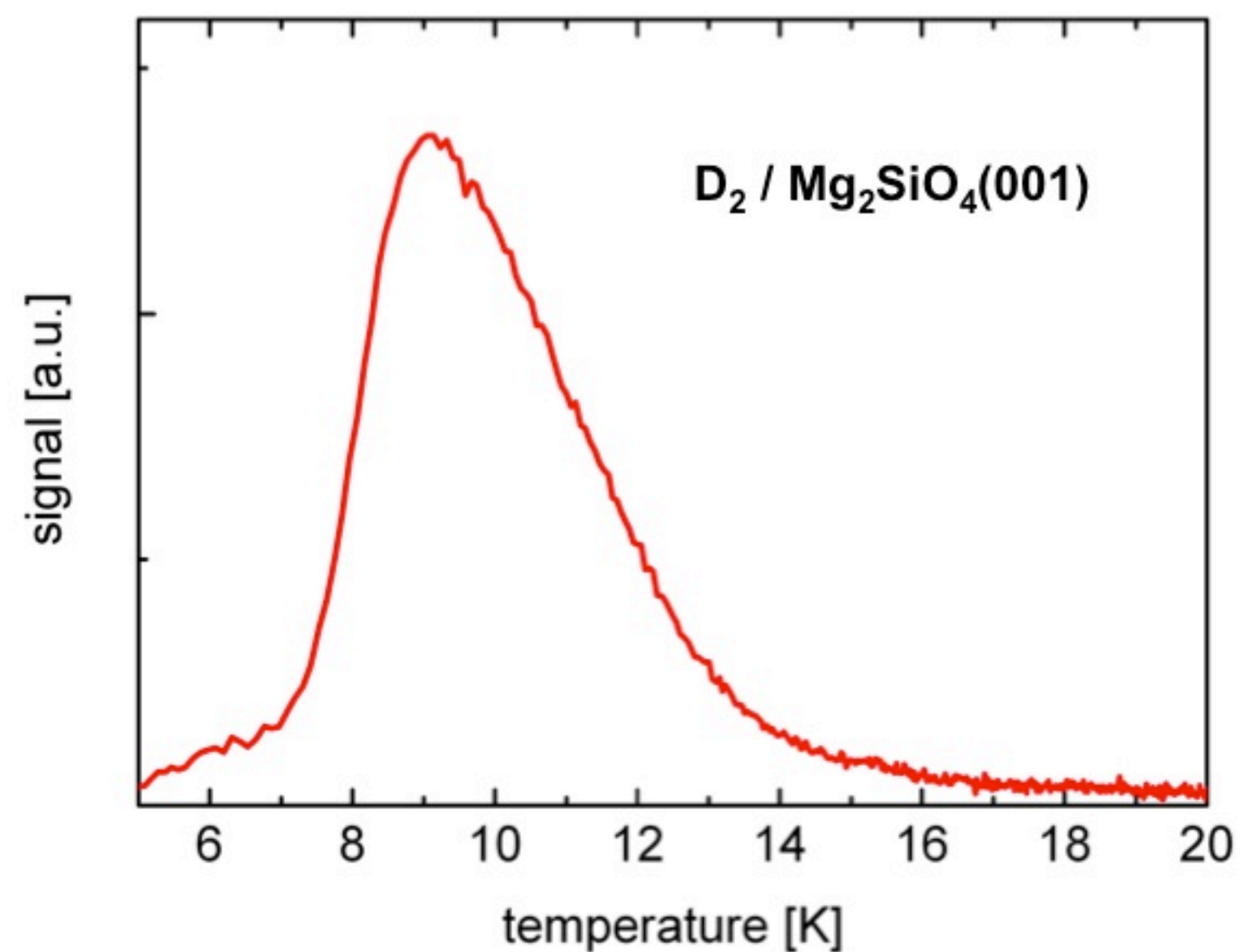
Ice formation



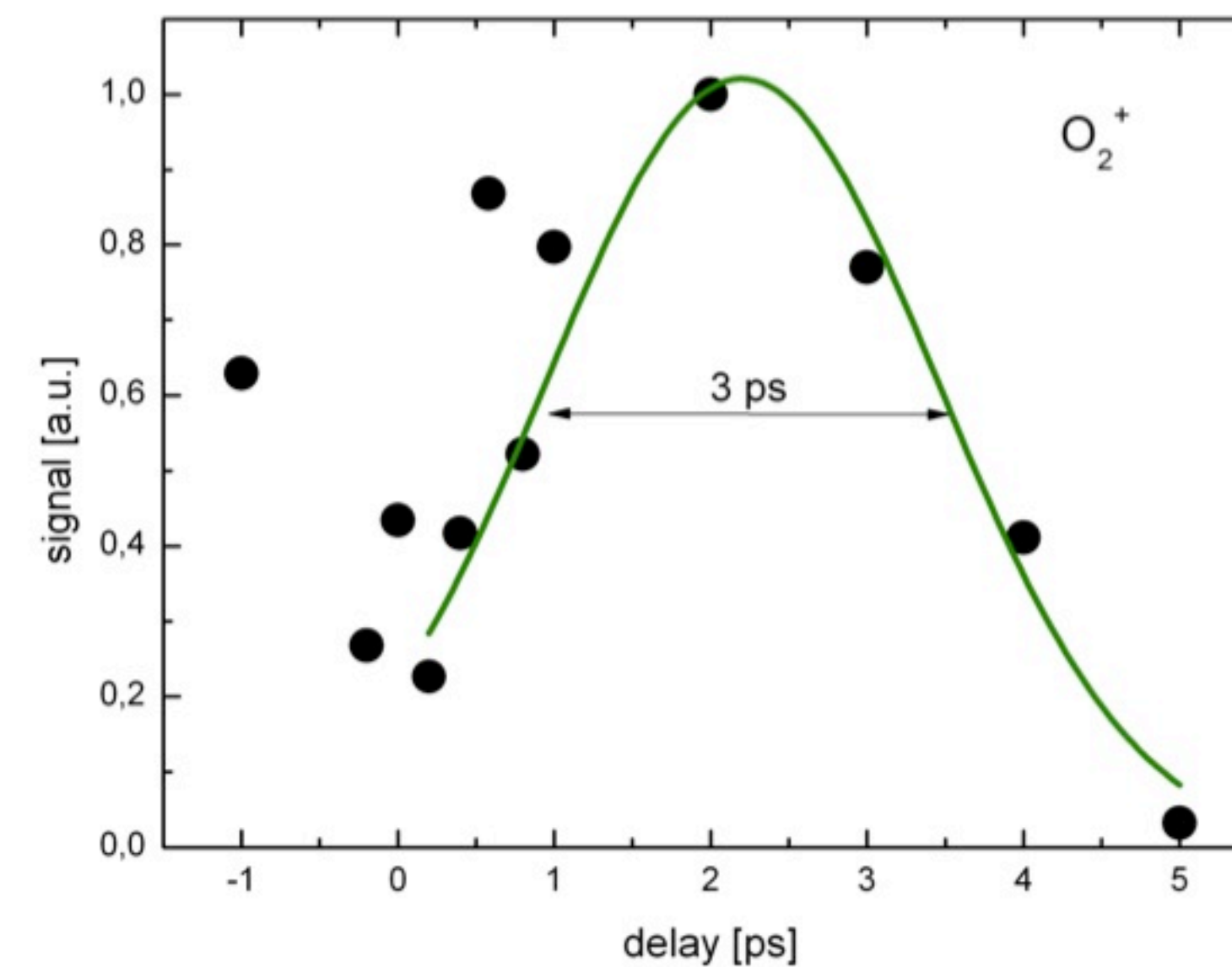
Ice particle break-up



Thermal desorption



XUV photochemistry



Peer reviewed articles

1. Desorption of ionic species from ice/graphite by femtosecond XUV free-electron laser pulses
B. Siemer, T. Hoger, M. Rutkowski, R. Treusch, H. Zacharias
J. Phys.: Condens. Matter **22**, 084013 (2010)
2. Desorption of H atoms from graphite(0001) using XUV free electron laser pulses
B. Siemer, T. Olsen, T. Hoger, M. Rutkowski, C. Thewes, S. Düsterer, J. Schiøtz, H. Zacharias
Chem. Phys. Lett. **500**, 291 (2010)
3. Site specificity in femtosecond laser desorption of neutral H atoms from graphite(0001)
R. Frigge, T. Hoger, B. Siemer, H. Witte, M. Silies, H. Zacharias, T. Olsen, J. Schiøtz
Phys. Rev. Lett. **104**, 256102 (2010)
4. XUV free-electron laser desorption of NO from graphite (0001)
B. Siemer, T. Hoger, M. Rutkowski, S. Düsterer, H. Zacharias
J. Phys. Chem. A **115**, 7356 (2011)
5. Breaking the Ice: Planetesimal Formation at the Snowline
G. Aumatell and G. Wurm
MNRAS, in press, 2011
6. Thermal desorption spectroscopy of small molecules from natural olivine
N. Heming, B. Siemer, H. Zacharias,
in prep.

Conferences

Conference contributions

1. G. Aumatell and G. Wurm, First Observations of mm and sub-mm Ice Aggregation, Planet Formation and Evolution, Göttingen, 2011
2. G. Aumatell and G. Wurm, Collisions of (sub-)mm size Ice Aggregates, EPSC-DPS Joint Meeting, Nantes 2011
3. G. Aumatell and G. Wurm, Collisions of (sub-)mm size Ice Aggregates, The Chemical Cosmos, Malta 2011
4. B. Siemer, M Wöstmann, R. Frigge, R. Mitzner, H. Zacharias, Non-linear surface chemistry with XUV radiation from FLASH, FLASH II Meeting, Hamburg, 2011

Contributions to LASSIE related events

1. G. Aumatell and G. Wurm, Dust and Ice Aggregation in Protoplanetary Disks, LASSIE & Astrophysical Chemistry Group: Young Researchers Meeting, London, October 2010
2. G. Aumatell and G. Wurm, First Observations of mm and sub-mm Ice Aggregation, LASSIE Training Leiden, 2011
3. G. Wurm, Laboratory Experiments on Free Ice Particles in the Context of Planetesimal Formation, Astrosurf Meeting, Edinburgh 2011.
4. G. Aumatell and G. Wurm, Breaking the Ice: Planetesimal Formation at the Snow Line, Astrosurf Meeting, Edinburgh 2011.
5. B. Siemer, N. Heming, M. Wöstmann, R. Mitzner, H. Zacharias, Desorption processes of XUV irradiated H and D₂O covered graphite surfaces with FLASH, Astrosurf Meeting, Edinburgh, 2011



Career Development

Training: Active participation in several activities by G. Aumatell

first participation by T. Susaharia

Placement: G. Aumatell: planned at Universit of Strathclyde (Dr. Fraser, Scotland)

T. Susaharia: not decided yet

Outreach

Astroseminar 2011

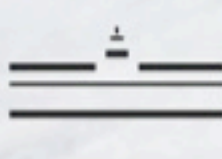


Entstehung und Entwicklung von Planetensystemen und mögliches Leben

Wann? 21. und 22. Oktober 2011
Was? Spannende und interessante Vorträge über grundlegende und aktuelle Themen.
Wer? Alle Interessierte! Keine Vorkenntnisse erforderlich.
Wieviel? Der Eintritt ist frei.
Wo? Institut für Kernphysik
Wilhelm-Klemm-Str. 9, 48149 Münster

www.uni-muenster.de/Astroseminar

Das Astroseminar wird unterstützt von:
Deutsche Physikalische Gesellschaft / WE-Heraeus-Stiftung, Fachbereich Physik der WWU, LASSIE FP7 ITN, Universitätsbuchhandlung Krüper, Spektrum Verlag, Wiley-VCH Verlag



WESTFÄLISCHE
WILHELMS-UNIVERSITÄT
MÜNSTER



Programm

- Bartelmann:** Risiken und Nebenwirkungen des Urknalls
- Rauer:** Entdeckung und Charakterisierung extrasolarer Planeten
- Biermann:** Die ersten Sterne und die ersten dicken schwarzen Löcher
- Weinheimer:** Kalte dunkle Materie und Strukturbildung
- Wurm:** Die Entstehung von Planetensystemen in ihrer frühen Phase
- Spohn:** Leben und Entwicklung von Planeten

plus talks from **Graduate Students**



Research

- First **growth of ice aggregates** in collisions has been observed (to be continued)
- **Sublimation and break-up of ice aggregates** has been analyzed (to be continued)
- Thermal desorption of various molecules from **olivine** and **forsterite(001)**
- First **XUV photochemistry** in pure water ice
- Numerous contributions to **conferences** and **first papers**

Summary

Ice formation: project evolves steadily as planned

Photochemistry: late start of the ESR,
but the scientific and training deliverables will be met

Max-Planck-Gesellschaft

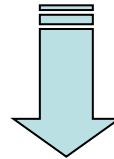


Max Planck Institute for Astronomy in Heidelberg, Germany



96 person months

2 ESRs (72 Person-Months) first tranche,
1 ESR (24 Person-Months) second tranche



Tolou Sabri (36 pm):

Experimental study on condensation and processing of dust in Astrophysical Environments

Supervisor: C. Jäger,
Th. Henning

WP1

Tobias Albertsson (36 pm):

Isotopic fractionation and complex chemistry in the ISM and protoplanetary disks

Supervisor: D.Semenov,
Th. Henning

WP4

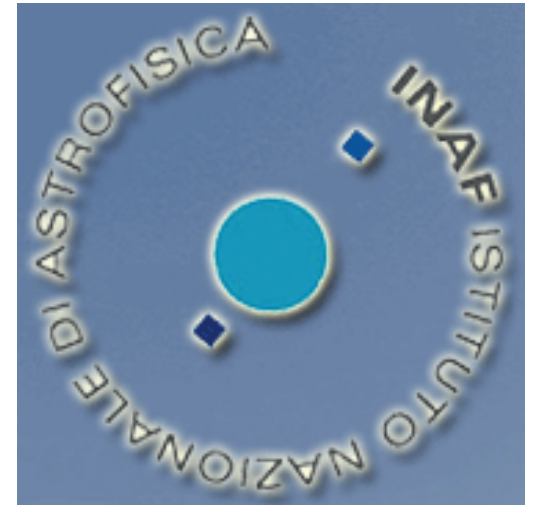
Siyi Feng (24 pm):

Chemical sub-structure of high-mass star-forming regions

Supervisor: H. Beuther,
Th. Henning

WP5

National Institute for Astrophysics



INAF-CATANIA ASTROPHYSICAL OBSERVATORY

LABORATORY OF EXPERIMENTAL ASTROPHYSICS

STAFF:

M.E. PALUMBO

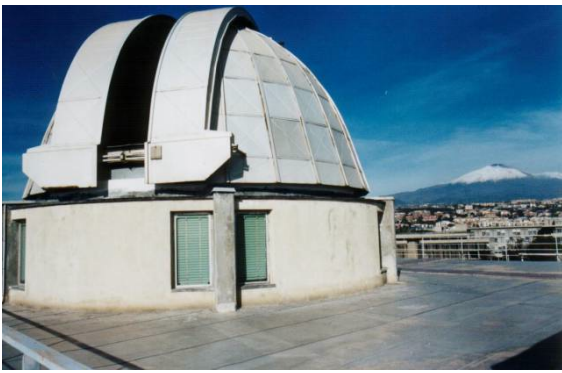
G. BARATTA

G. LETO

G. STRAZZULLA

STUDENTS, PHD, FELLOWS,

Z. KANUCHOVA, I. SANGIORGIO, F. ISLAM



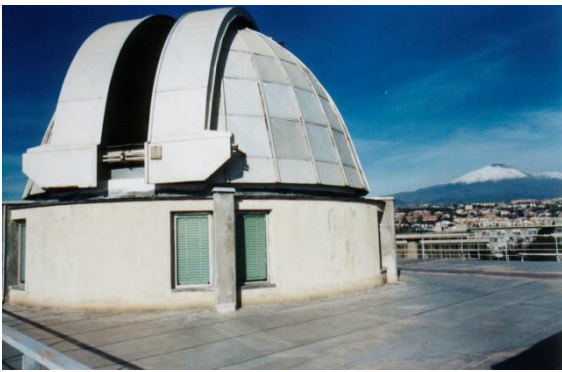
COLLABORATIONS



UCL: Angela Occhiogrosso (ESR), Serena Viti

MPI fuer Astronomie Jena: Tolou Sabri and
Cornelia Jager

Strachclyde University: Aleksu Suutarinen and
Helen Fraser



Role in LASSIE



- Lead WP3 “Chemical transformations in and on icy grains
- Organization of the first Training School on Astrochemistry with ALMA. Bologna, 13-17 June 2011

Leiden University

Leiden University

Pathways towards Molecular Complexity in Space

-The solid state laboratory approach –

*Laboratory for Astrophysics, Leiden Observatory
The Netherlands*

Steven Cuylle, ESR

Gleb Fedoseev, ESR

Irene San Jose Garcia, ESR

Ewine van Dishoeck, PI

Harold Linnartz, PI



Pathways towards Molecular Complexity in Space

-The solid state laboratory approach –

*Laboratory for Astrophysics, Leiden Observatory
The Netherlands*

Five ice experiments

*SURFRESIDE, CRYOPAD, MATRIICES,
OASIS, HV setup*

Astronomical observations



Pathways towards Molecular Complexity in Space

-The solid state laboratory approach –

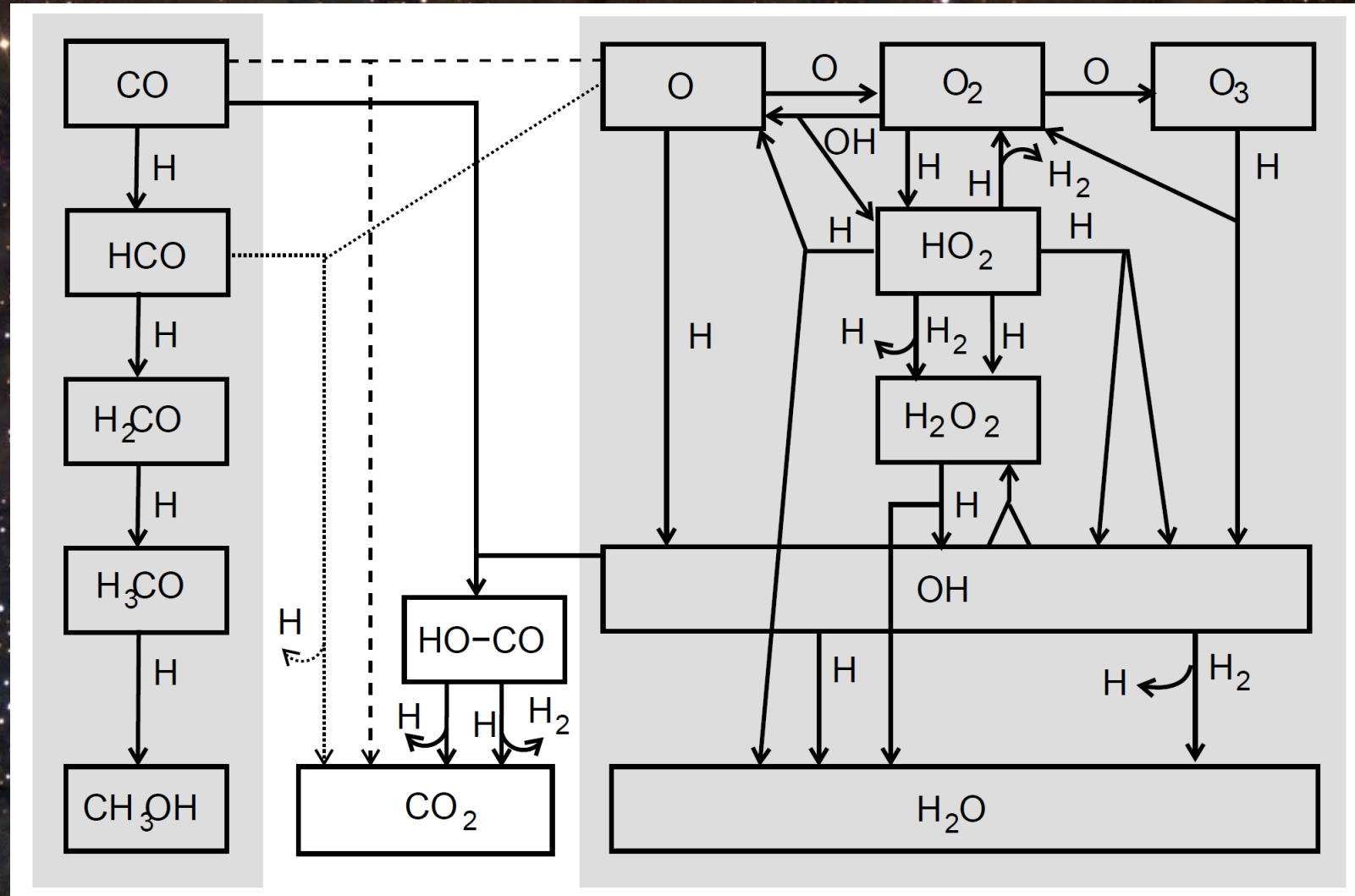
*Laboratory for Astrophysics, Leiden Observatory
The Netherlands*

*Spectroscopy and reaction dynamics of
interstellar ice analogues*

*Analytical observations to characterize
gas grain interactions*



Atom addition reactions



Photoprocessing of ices

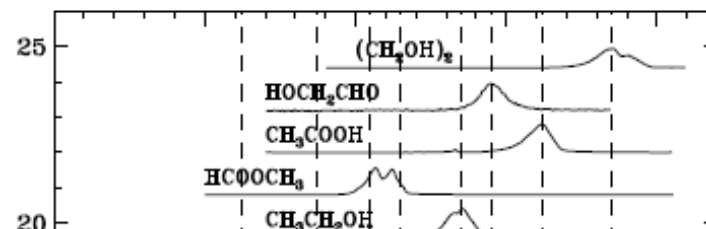
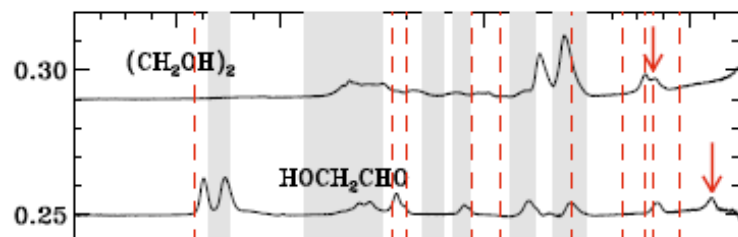
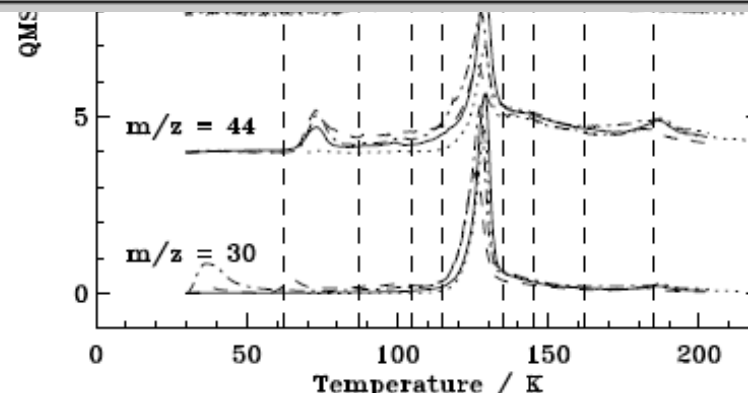
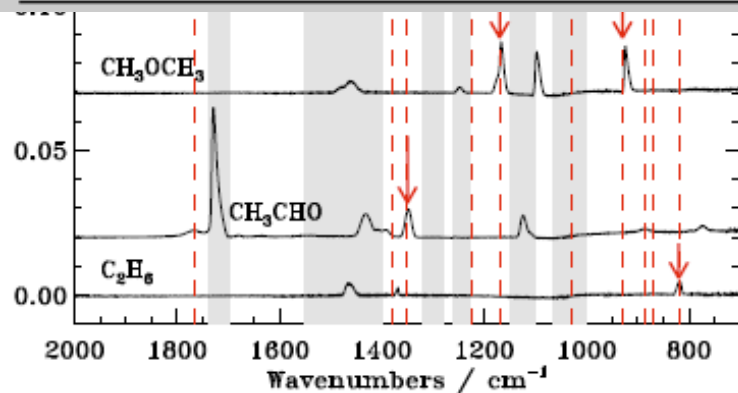
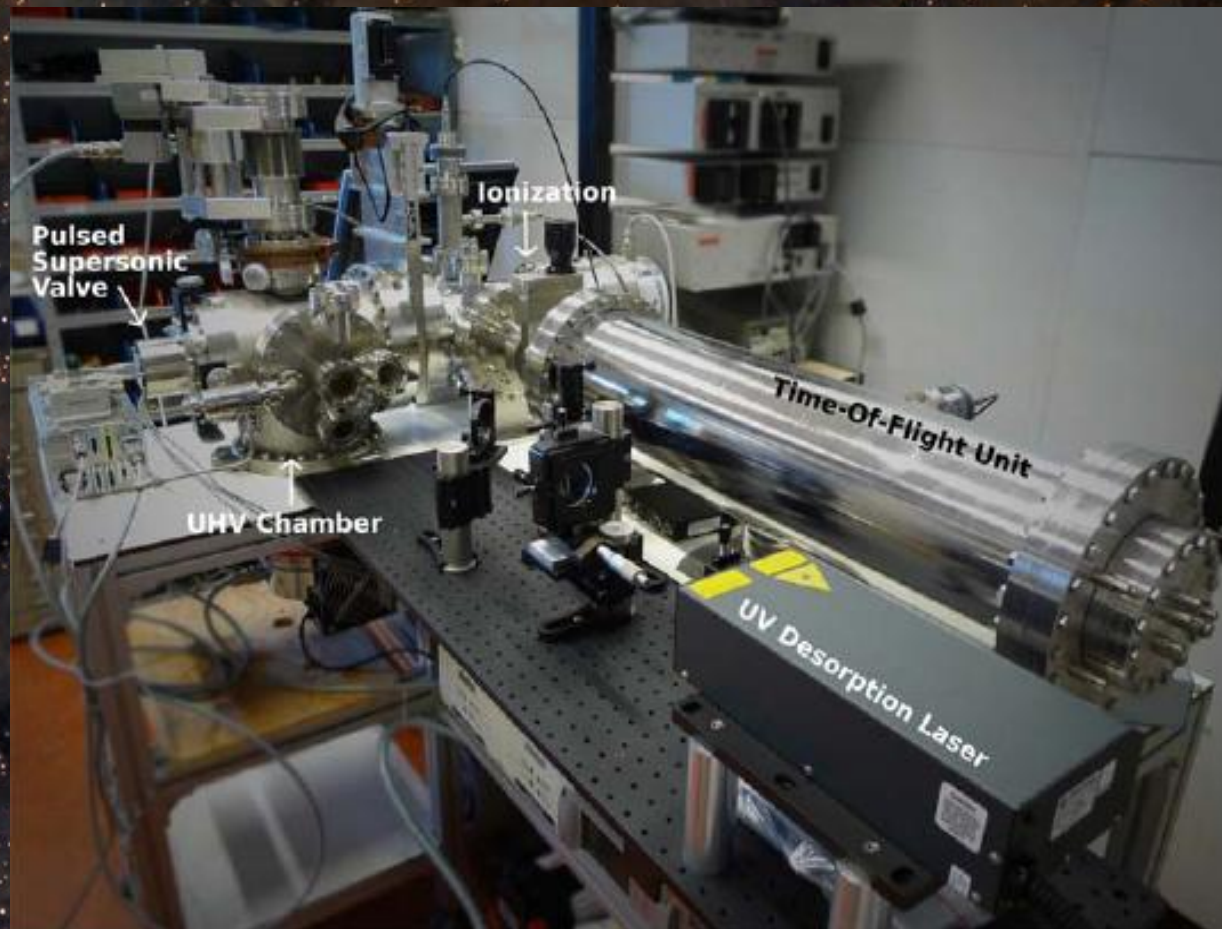


Table 6. Abundances of complex molecules relative to CH₃OH.

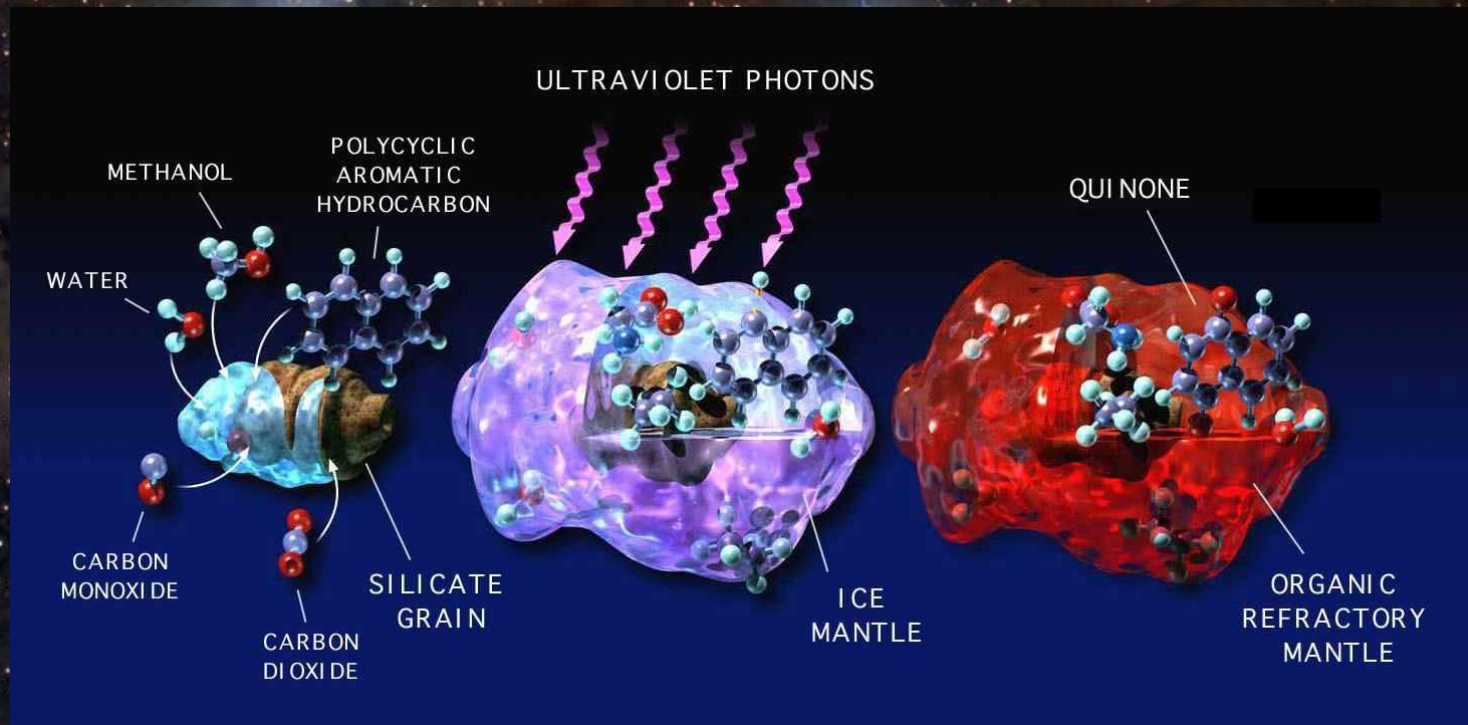
	IRAS 16293-2422/A ^{a,b}	Hot cores ^c	L1157 ^d	MC G-0.02 ^e	Hale-Bopp ^f	CH ₃ OH ^g	CH ₃ OH:CO ^g
CH ₃ OH	1/1	1	1	1	1	1	1
CH ₃ CHO	0.038/ < 0.0016	2.9[3.1] × 10 ⁻⁵	–	0.033	0.010	0.01	< 0.04
CH ₃ CH ₂ OH	~0.031	0.019[0.012]	0.007	0.040	< 0.042	0.1	< 0.01
CH ₃ OCH ₃	0.20/0.013	0.41[0.51]	–	0.050	–	0.04	< 0.01
HCOOCH ₃	0.30/0.0084	0.089[0.084]	0.019	0.037	0.033	< 0.03	> 0.08
HOCH ₂ CHO	–	–	–	0.01	< 0.017	< 0.04	> 0.04
(CH ₂ OH) ₂	–	–	–	0.01	0.10	0.4	< 0.01



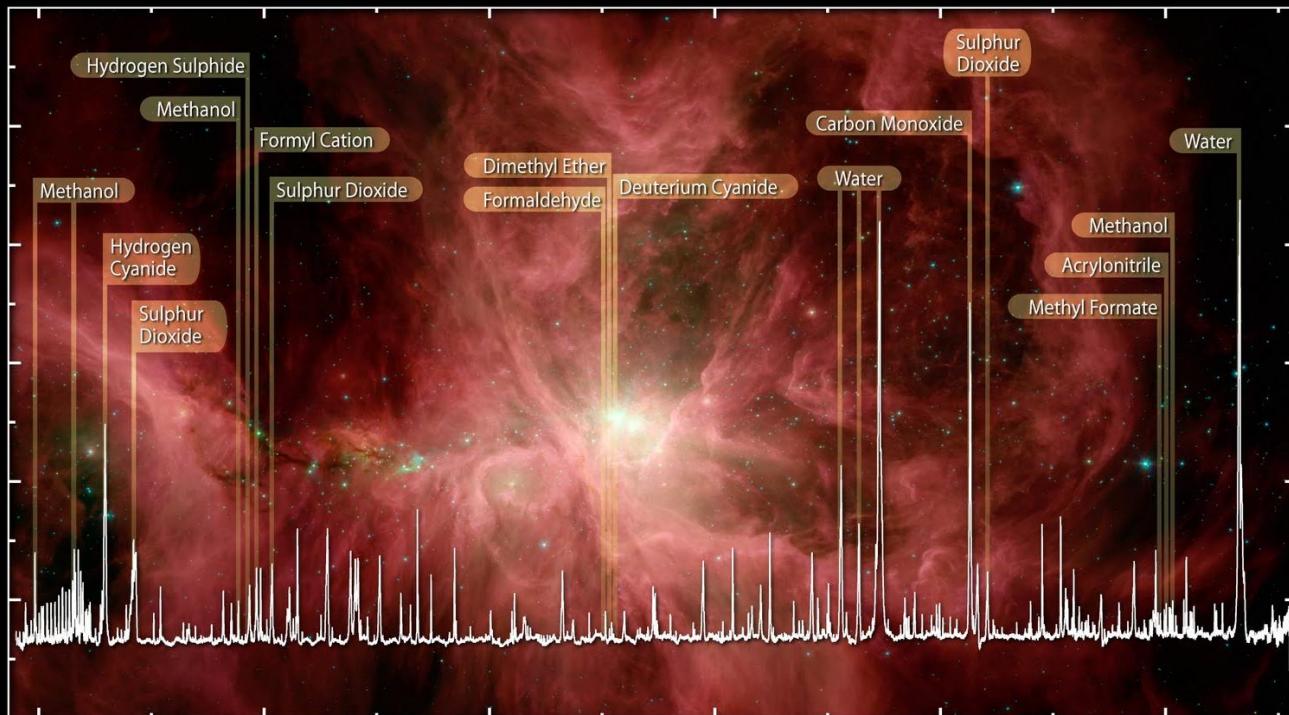
Towards 'real' molecular complexity in interstellar ice



Towards 'real' molecular complexity in interstellar ice



The astronomical link



HIFI Spectrum of Water and
Organics in the Orion Nebula

© ESA, HEXOS and the HIFI consortium
E. Bergin

Chalmers University

Gothenburg,
Sweden's second largest
with 500 000 inhabitants

CHALMERS

University of Technology



Areas of advance

Chalmers has eight areas of advance where the aim is to bring together research, education and innovation across departmental boundaries and to co-operate with bodies and organisations outside Chalmers.

- Built Environment
- Energy
- Information and Communication Technology
- Life Science
- Materials Science
- Nanoscience and Nanotechnology
- Production
- Transportation

The eight key areas also have a firm foundation in the basic sciences. Sustainability, innovation and entrepreneurship are strong driving forces.

Major Research Infrastructures



Nanofabrication Laboratory

A state-of-the-art cleanroom facility
European transnational access facility



Onsala Space Observatory

A national research facility for
advanced radio astronomy

Students

First degree and Master's programmes

Chalmers has about 11,000 students (individuals)

1,720 students in BScEng and BSc Programmes (full-time equivalents)

- 281 degrees awarded 2010

3,295 students in MScEng and MArch Programmes (full-time equivalents)

- 727 degrees awarded 2010
- 22 International MSc degrees awarded 2010



Students

Doctoral programmes

1,130 doctoral students

243 degrees awarded 2010

- 121 PhDs
- 122 licentiates



Staff

2,493 employees (full-time equivalents)

- 1,751 teaching and research staff
- 742 technical support and administrative staff

Scientific Articles

- More than 1,900 peer reviewed scientific articles and conference contributions



European collaborations

– some examples

- 140 EU-projects and other European projects
- European transnational access facility
(the Nanofabrication Laboratory)
- Erasmus Mundus Master's programmes in
Nanoscience and Nanotechnology

Department of Applied Physics

is the largest individual physical environment in Gothenburg

- **200 teachers and researchers**
- **120 PhD students**
- **550 undergraduate students.**

University of Gothenburg

University of Gothenburg



The UGOT team

PI:	Gunnar Nyman	
LASSIE ER:	Dr. Dylan Drake Wilhelm	July 2010
LASSIE ESR:	Bethmini Senevirathne	Sept 2010
LASSIE ESR:	Pavel Elkind	2012
Researcher:	Dr. Stefan Andersson	

Collaboration: Helen Fraser, Strathclyde

Theme 4:

Modelling the gas-grain interaction

Theme 1 - Formation of Grains, Small Molecules and Ices

Theme 2 - Physical Processes in and on Icy Grains

Theme 3 - Chemical Transformations in and on Icy Grains

Theme 4 - Modelling the Gas-Grain Interaction

Theme 5 - Observations and Astronomical Models Involving Dust and Ices

Topics:

- Hydrogen molecule formation on interstellar ices (Bethmini, Gunnar, Stefan)
- Photochemistry of interstellar ices (Dylan, Gunnar, Stefan)

University College London

LASSIE

PI: Steve Price, Chemistry

Reactive species on surfaces

UCL- CCCP

Jonathan Rawlings, Physics

Protostar formation, observations

Serena Viti, Physics &
Astronomy

Star formation, desorption

Processes on Dust Grains

Daren Caruana, Chemistry

Astro-electrochemistry

Mike Barlow, Physics

Evolved Stars, Planetary Nebulae

Wendy Brown, Chemistry

Desorption processes; molecular formation

David Williams, Physics

H₂ formation, star formation

Fabrizio Puletti – Chemistry (supervisor Wendy Brown/Steve Price)

Experimental studies of desorption and molecular formation
of S-species

Angela Occhiogrosso – Physics & Astronomy (supervisor Serena Viti/Wendy Brown)

Development of surface reaction networks in astrochemical models
of star forming regions

Other researchers

Chemistry – Mark Whelan (student); Michael Ward (student);
Daren Burke (PDRA)

Physics & Astronomy – Hannah Calcutt (student); Helen
Christie (student); Paul Woods (PDRA)

- Molecular formation on grains studied by RAIRS/TPD and REMPI (theme 1 - Chemistry)
- Studies of thermal desorption of pure and mixed ices (theme 2 - Chemistry)
- UV and electron processing of ices (themes 1, 2, 3 - Chemistry)
- Astronomical observations of evaporated ices in different environments using e.g. JCMT, Herschel (theme 5- Physics & Astronomy)
- Modelling of gas-grain chemistry in hot cores and comparing with observations (theme 5 – Physics & Astronomy)
- Direct collaboration between Physics and Chemistry and Catania to look at sulphur chemistry in ices using experiments and modelling

The Open University



OPEN UNIVERSITY

Professor Nigel Mason



The Open University



Open University role



Outreach coordination

- **Employ and train two ESRs**
- **Ewelina Szymanska** and **Binukumar G Nair**



Open University role



Ewelina Szymanska

Research project

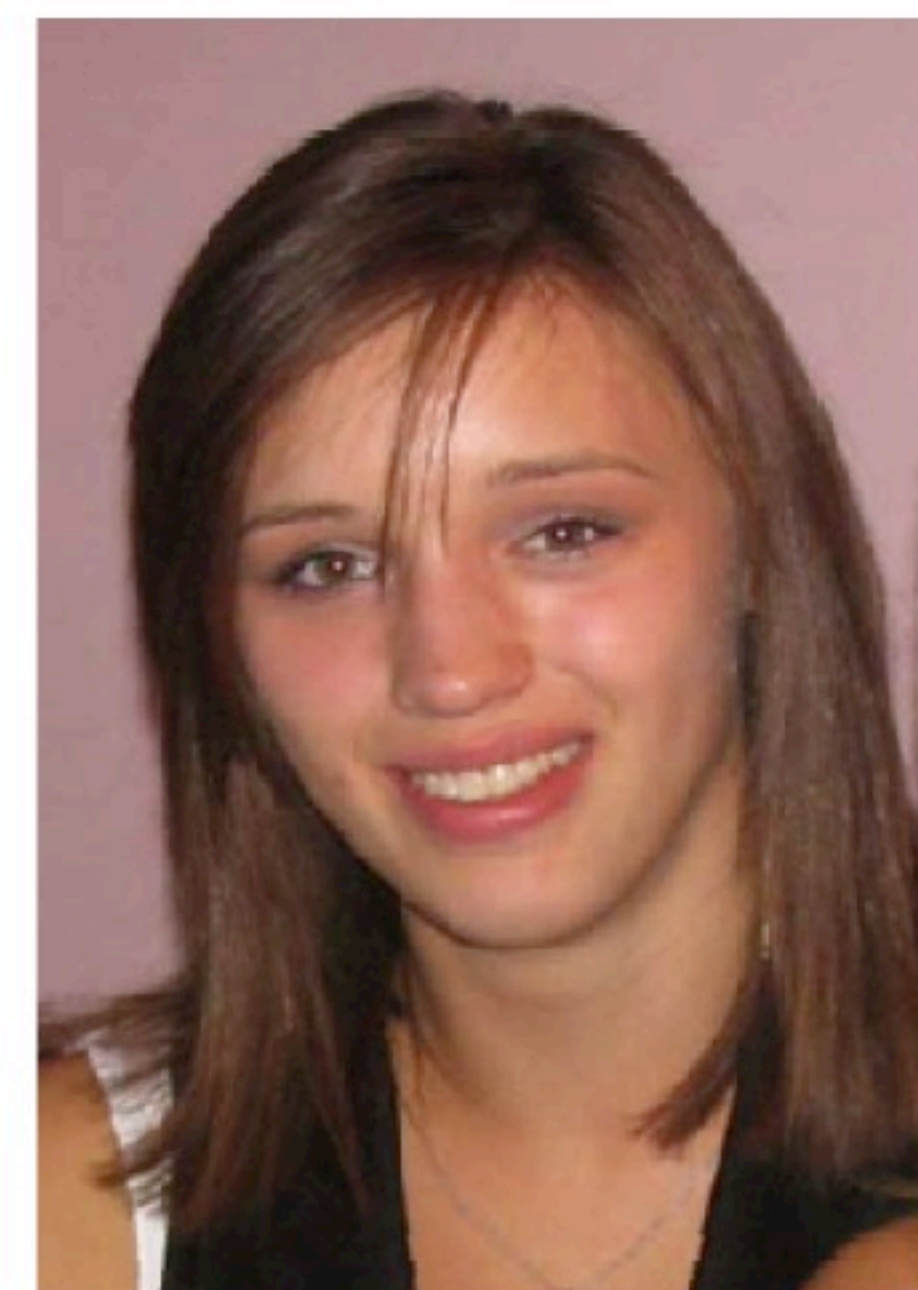
Exploring the electron induced chemistry in mimics of the icy surfaces on dust grains in the interstellar medium.

Relates to Theme 2 of the ITN

Understanding desorption of simple ices, complex mixed ices and clathrates induced through interaction with electromagnetic radiation and Understanding desorption of simple ices, complex mixed ices and clathrates induced *via* interaction with low energy electrons and models of cosmic rays and

Theme 3 of the ITN UV photon- and low energy electron-induced chemical transformations.

This work links to Queens Belfast where similar experiments will be performed using ion beams as the irradiation source





Open University role



Binukumar G Nair
Research project

In accord with **theme 1**, To study the infrared, optical and ultraviolet (UV) spectroscopy of ices formed reactively on model dust grain surfaces

In accord with **theme 2**, To study the role of heat, electromagnetic radiation and cosmic rays in promoting changes in ice morphology and

In accord with **theme 3**, To study VUV, XUV and X-ray photon- and cosmic ray-induced chemical transformations



Cant be here today as French Consulate did not process/return Visa/passport in time

Queen's University, Belfast



Queen's University
Belfast



LASSIE - QUB

Tom Field*, Alan McLoughlin, Tom Millar**, Andra Muntean***

*Centre for Plasma Physics,

** Astrophysics Research Centre
School of Mathematics and Physics,
Queen's University Belfast,
Belfast BT7 1NN, N. Ireland, UK



LASSIE – Experiments- QUB

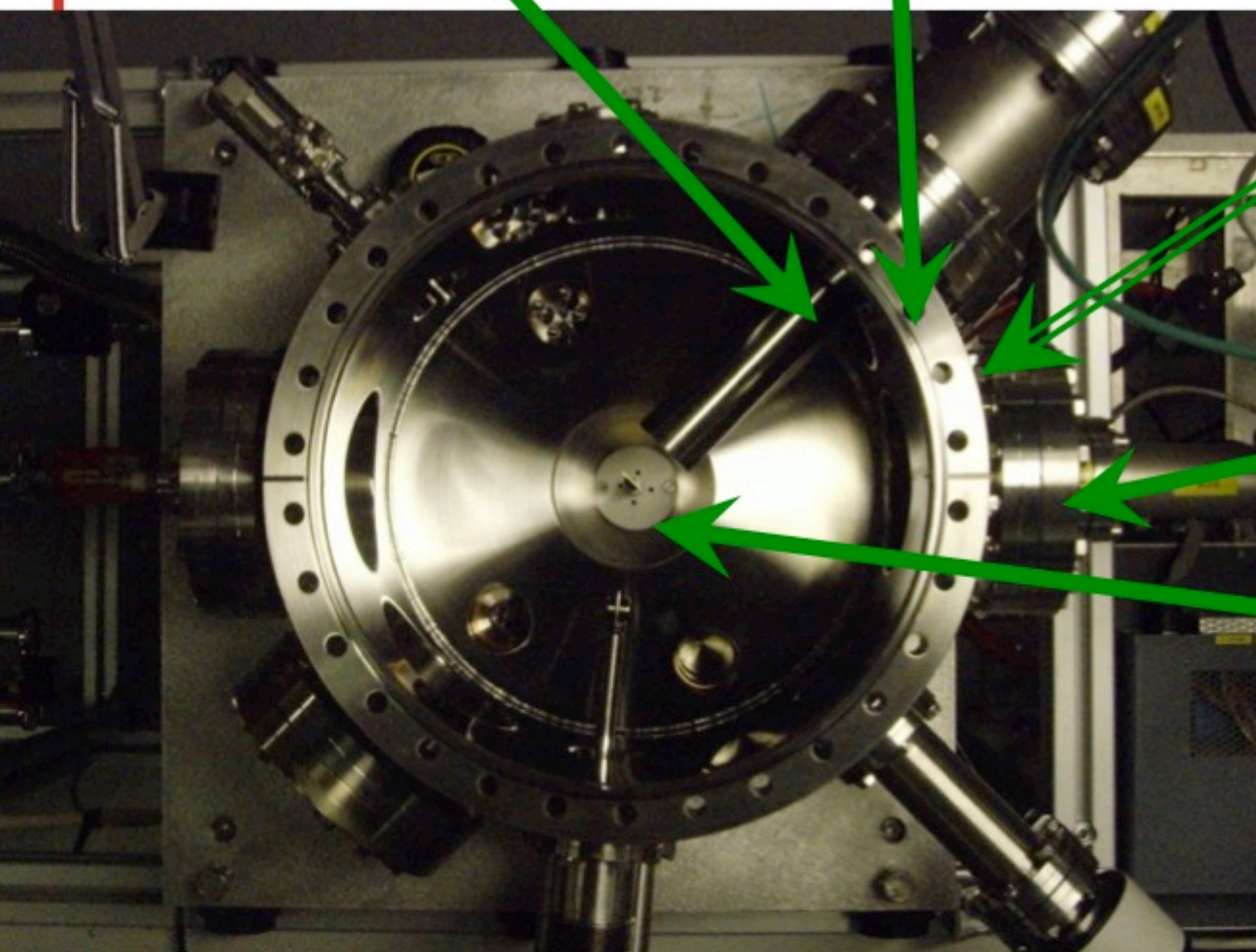
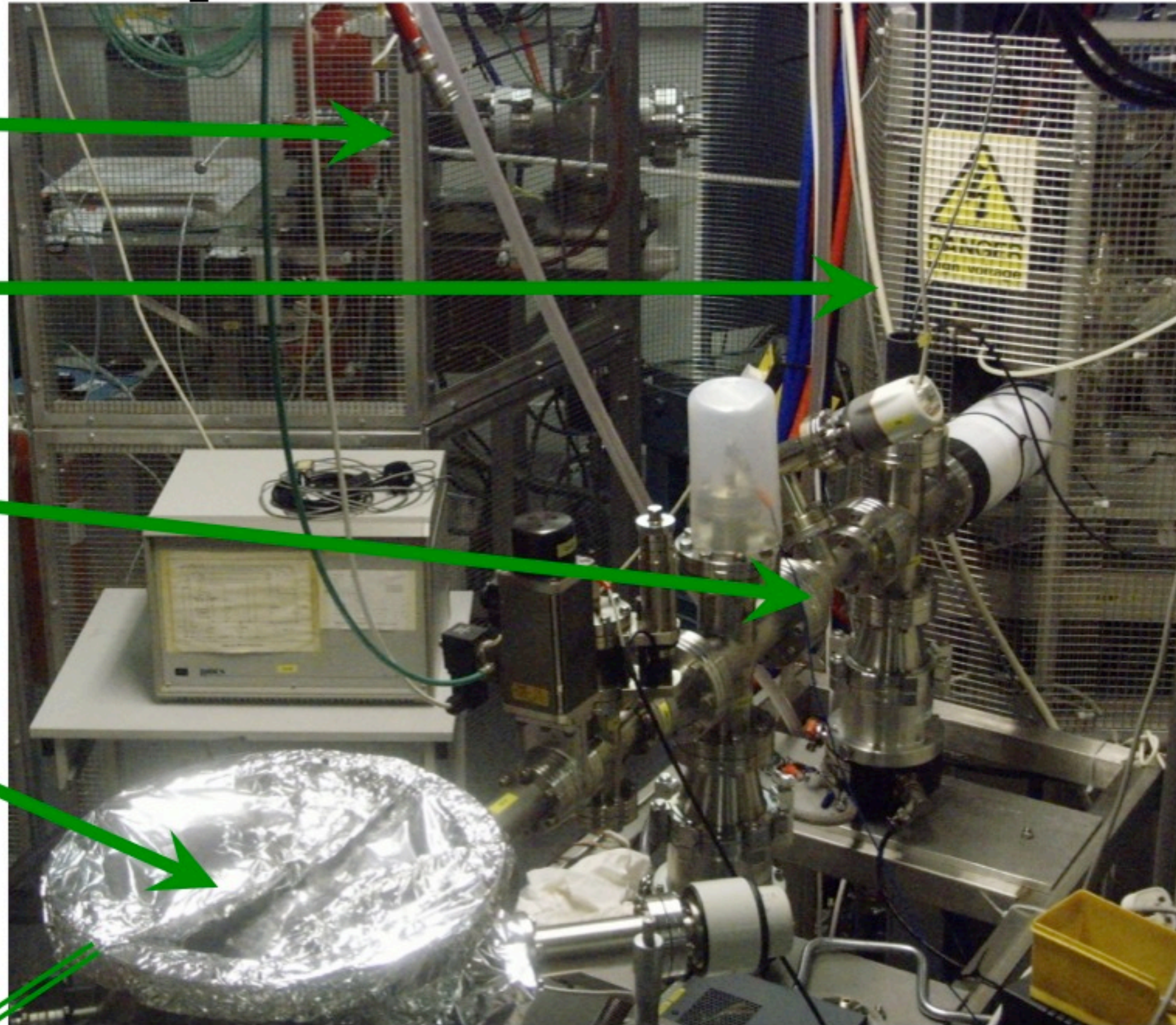
Ion source

Magnetic ion selector

Ion beamline

Target chamber

Quadrupole
Mass Spec



Ion beamline

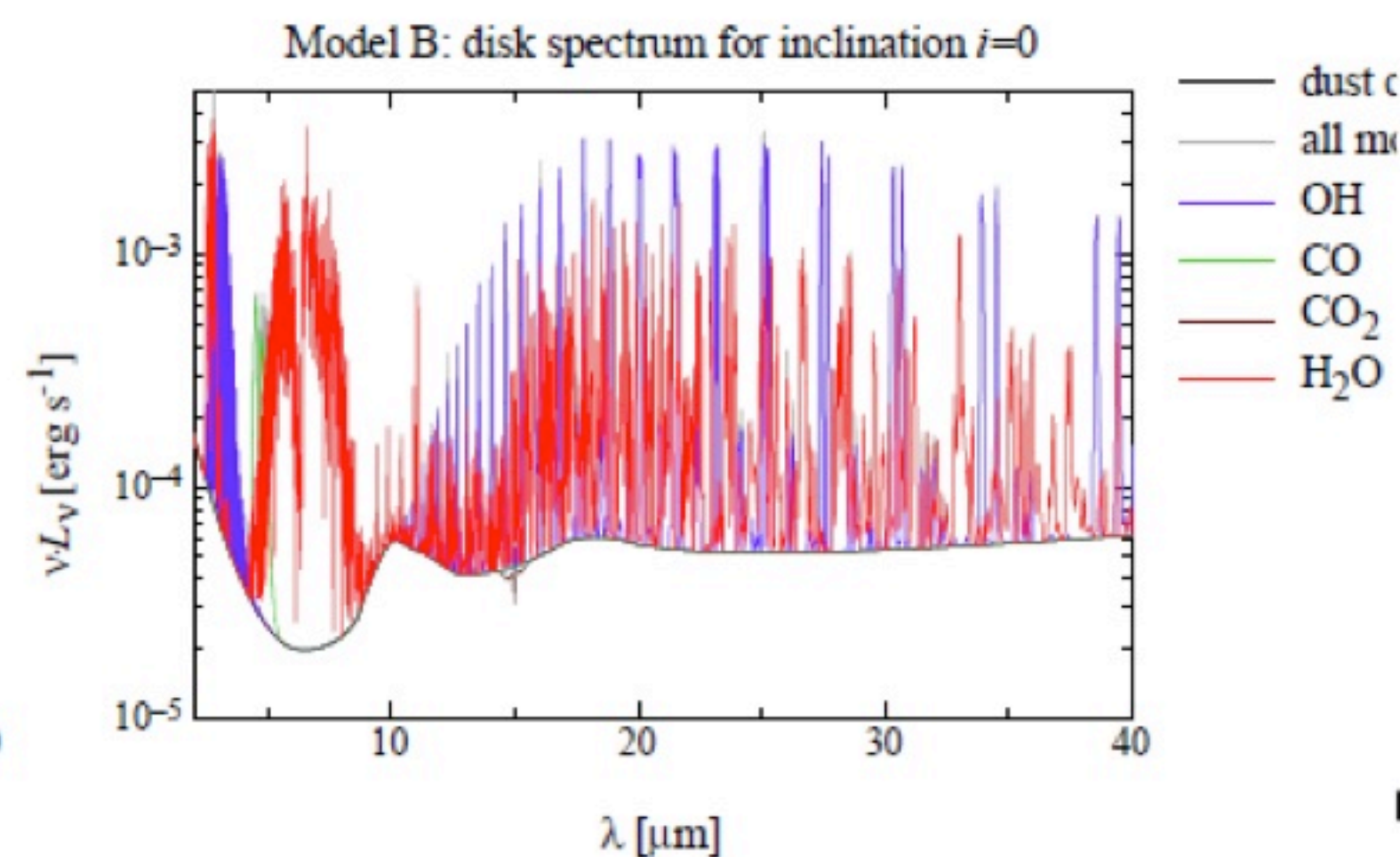
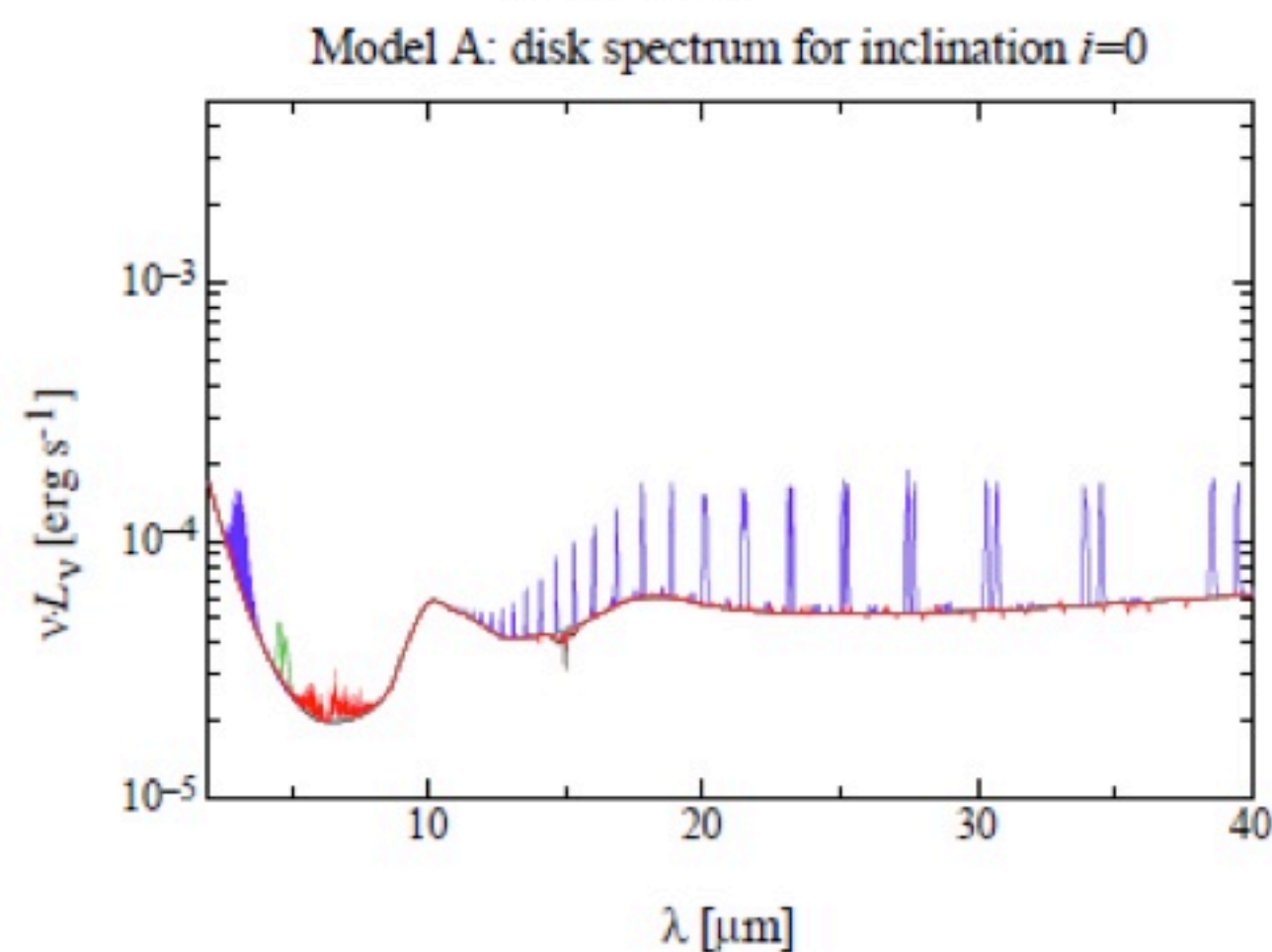
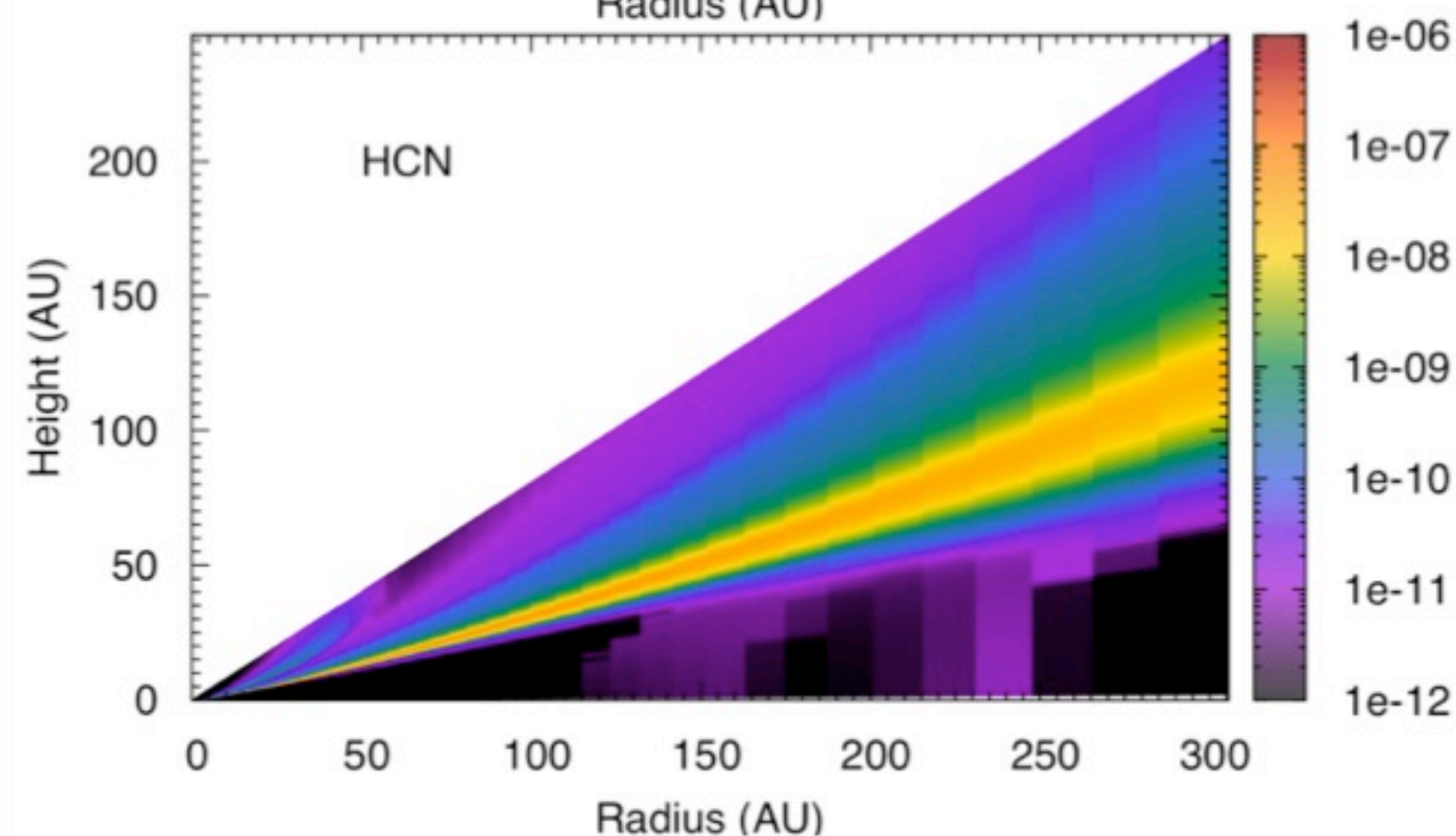
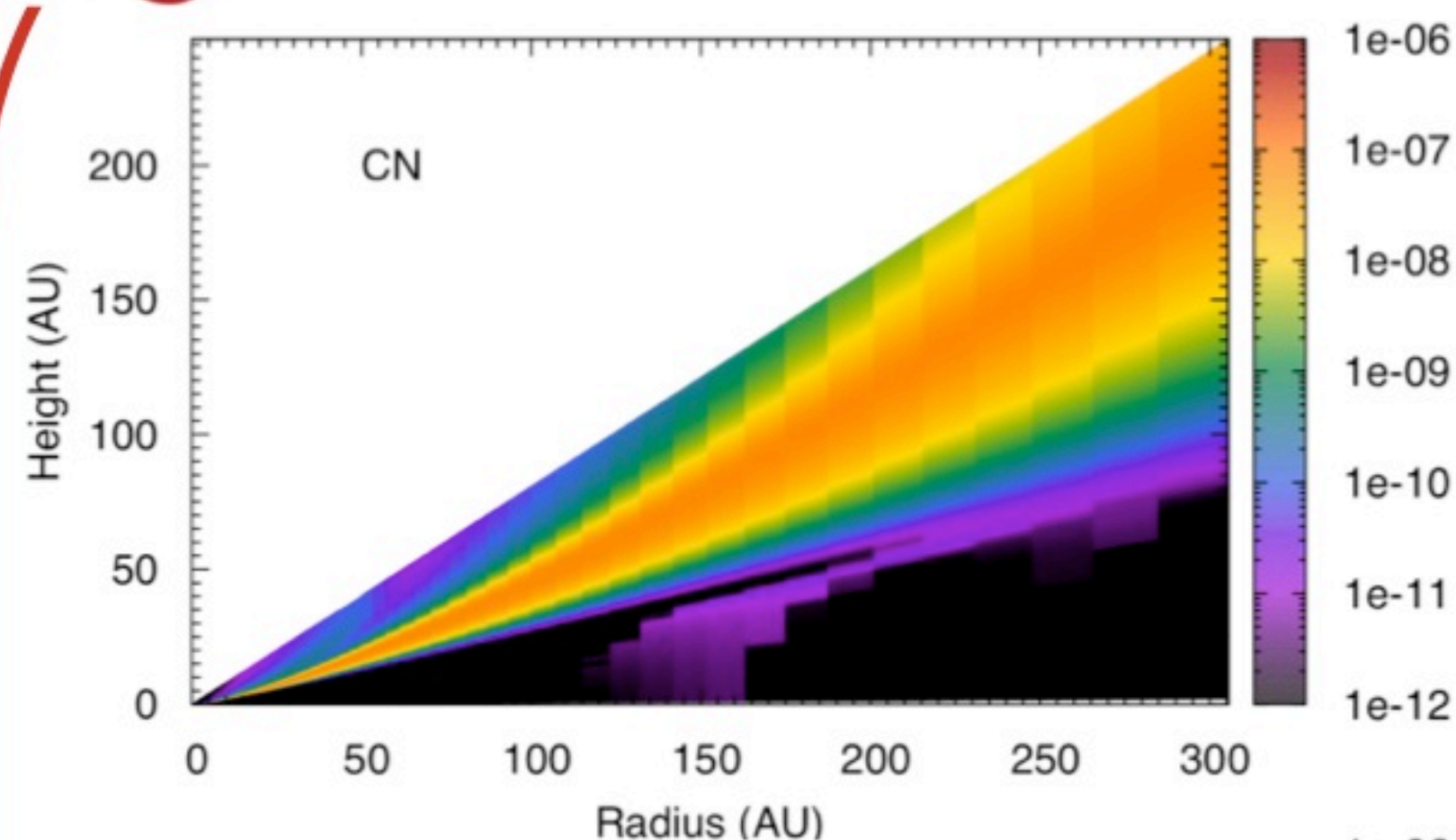
Target

Ice irradiation with keV energy ion beams of singly and multiply charged ions from ECR ion source. Analysis by SIMS and TPD with quadrupole mass spectrometer

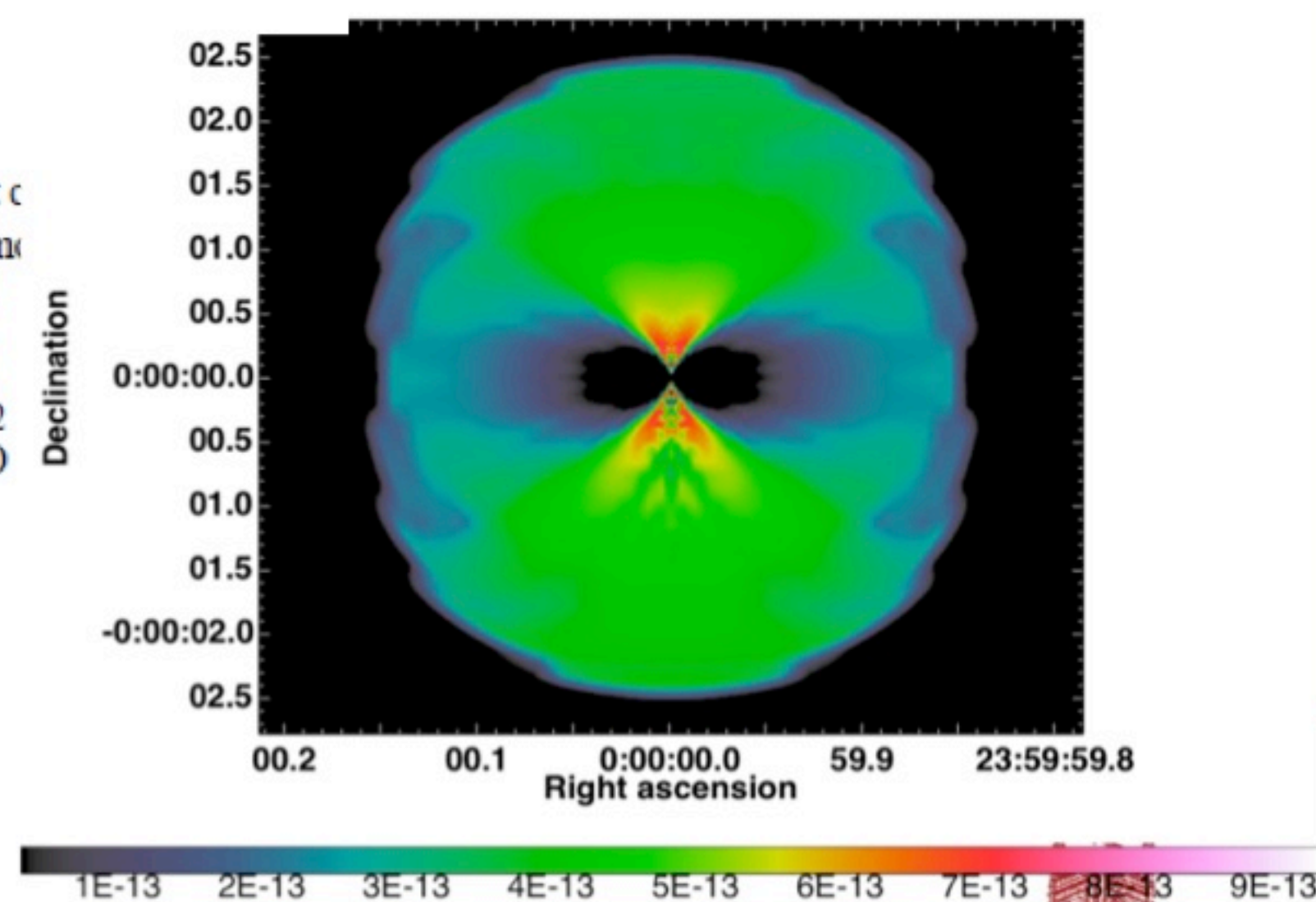


Molecular Astrophysics at Queen's

Modelling PPDs



ALMA



DM Tau



Strathclyde University



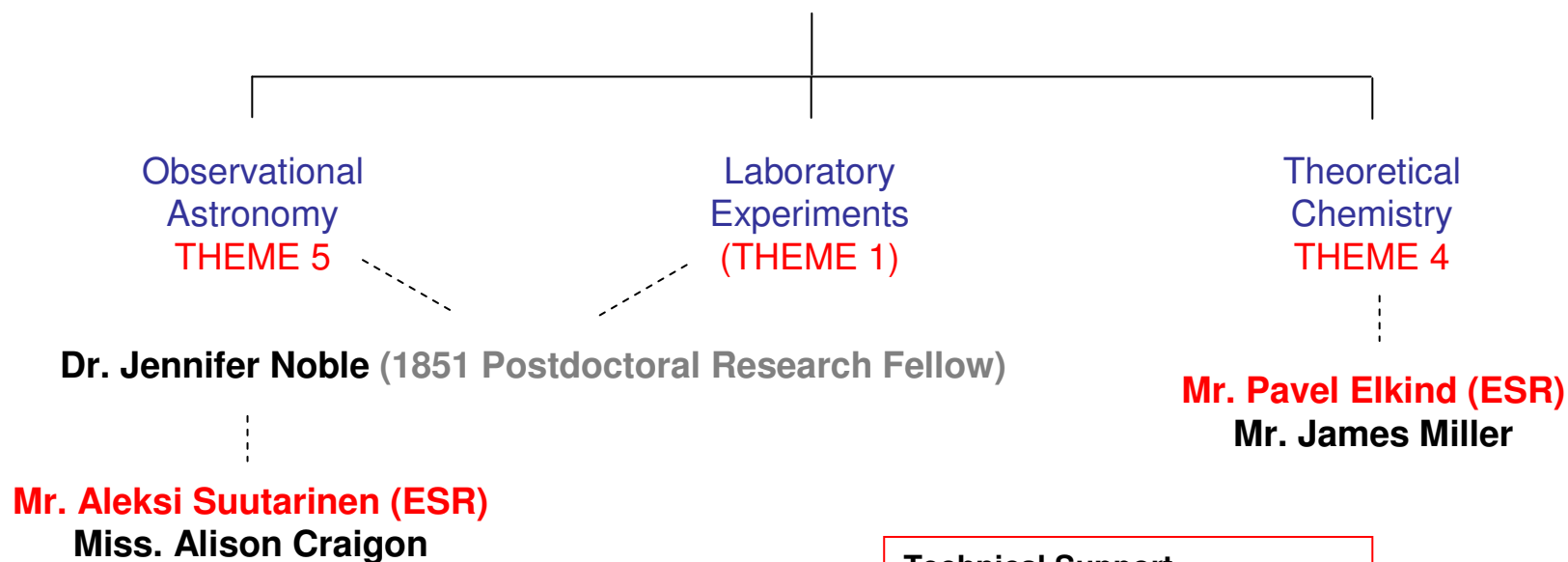
Overview

<http://astro.phys.strath.ac.uk>



Dr Helen Jane Fraser

academic leading research programme



Monday 14th November 2011
LASSIE –MTR
Fraser - Strathclyde

Technical Support

Mr. R.W. Dawson
Dr. R.Martin (HPC – Strathclyde)
Mr. T. Briggs



Astrochemistry





LASSIE Integration

<http://astro.phys.strath.ac.uk>



Dr Helen Jane Fraser

academic leading research programme

Observational
Astronomy
THEME 5

Mr. Aleksi Suutarinen (ESR)

Outgoing visit planned to
Leiden Observatory (EvD)
ESO Garching (EvD)

Laboratory
Experiments
(THEME 1)

Theoretical
Chemistry
THEME 4

Mr. Pavel Elkind (ESR)

Outgoing visit planned to
Gothenburg University (GN)



Monday 14th November 2011
LASSIE –MTR
Fraser - Strathclyde



Astrochemistry physics



Research



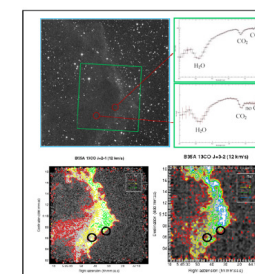
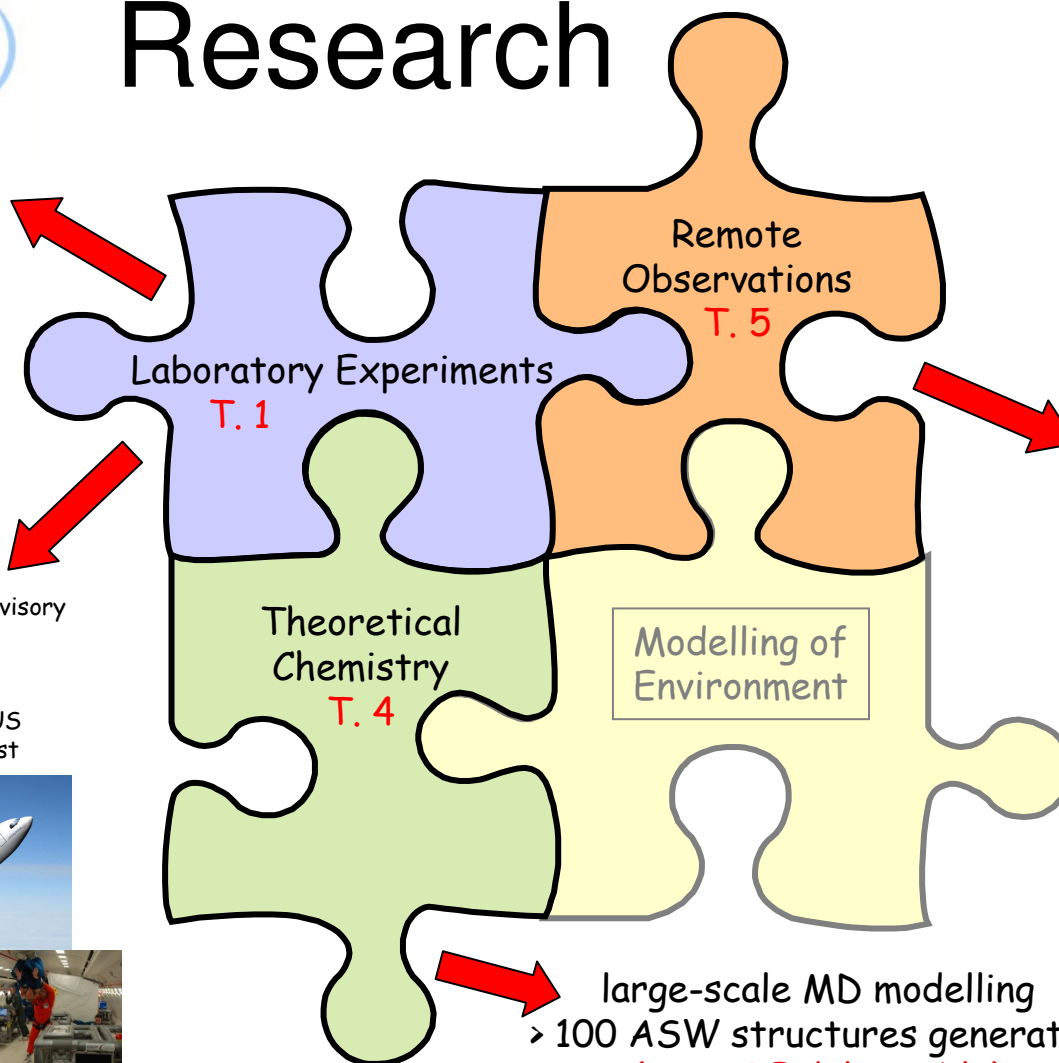
CO₂ Formation
Deuteration
Photochemistry

Noble et al ApJ (2011)
Thrower et al JVST (A)
(2008,2009)

Grain aggregation
(parabolic flight)

HJF appointed to UKSA ELIPS Advisory
Board on Microgravity

Uhrin et al (2011) MNRAS
Heisselman et al (2010) ICARUS
Salter et al (2009) Rev Sci Inst



Ice Mapping
(LASSIE deliverable)
Gas Depletion Mapping
1st confirmed detection
of D₂O (YSO / ISM)

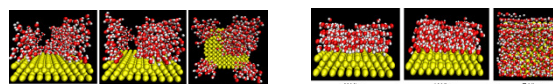
FRASER invited lecture
2nd International
AKARI Conference Korea (2012)

Noble et al (2009) PASP
Noble et al (2011) ApJ submitted
Craigon et al (2011a & b) A&A
submitted

FRASER invited lecture GRC
Computational Chemistry (2012)

Miller et al JCP (2011) submitted

large-scale MD modelling
> 100 ASW structures generated
(LASSIE deliverable)



Monday 14th November 2011
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Astrochemistry

<http://astro.phys.strath.ac.uk>





NEW Collaborations Internal Visits Expansion of work from Original LASSIE Remit



Dr Serena Viti (UCL)

LASSIE DELIVERABLE - *Herschel & JCMT Observations to Complete Gas-Ice Mapping of B35a*

Guillem Aumatell Gomez & Prof. Gerhart Worms Duisberg (ex - Munster)

Collisional Impacts of Icy Particles (Theory & Experiment)

Bethmini Senevirathne, Dr. Dylan Whyte / ER, Dr Stefan Andersson & Prof. Gunnar Nyman (Gothenburg)

LASSIE DELIVERABLE – *sharing MD structures for input to Photochemical MD model - over 100 structures so far*
Quantum Chemistry Calculations on Ice-Surface Reactions

Karoliina Isokoski, Harold Linnartz (Leiden Observatory)

Links between laboratory CH₃OH / CO / H₂O ice spectra & AKARI data

Experiments to test ice porosity, average and maximum height to cf with MD simulations

Lars Karssenmeijer, Dr. Herma Cuppen, (R.U. Nijmegen)

Prof. Marc van Hemert, Prof Ewine van Dishoeck, Universiteit Leiden

Sharing of CO-CO potential & CO-H₂O potential to incorporate into MD code & generate alternate ice models for
Applications in astrochemistry ice theory. NEW DELIVERABLE

Prof. Maria Elisabetha Palumbo (Catania)

CO₂ formation data @ grains surfaces – integration with AKARI data

Prof. David Field (Aarhus)

Calculation of residual z-dipole in MD formed ice structures for cf. with experiment

Prof. F. Duleiu, Dr. E. Congui (Cergy)

Experiments on Deuteration Of H₂O, linked to first detections of D₂O in interstellar objects (AKARI), CO₂ formation

Ex – LASSIE

Prof. Ant Jones (Observatoire de Paris)

Incorporation of latest C-H fitting data into AKARI data reduction of H₂O-ice band “red wing”

Dr Andreas Peterson (Reijkavik)

Path Integral Monte Carlo to study the meta-stability of MD ice structures

Prof. Thomas Loetering (Innsbruck)

Experimental neutron & Xray scattering to study ASW pore collapse & compare with MD simulations (ISIS / Diamond / ILL)



Monday 14th November 2011
LASSIE –MTR
Fraser - Strathclyde

**Aims for next 2 years =
Stronger links between AKARI ICE MAPPING +
ASTROCHEM MODELLING**

**Increase MD model size to observe
pore collapse & phase change**



Astrochemistry



<http://astro.phys.strath.ac.uk>