BENEFICIARY OF MEDEA

AARHUS UNIVERSITY

AARHUS

DENMARK

Address

Department of Chemistry, Aarhus University
Langelandsgade 140
DK-8000 Aarhus C – Denmark

Department of Physics and Astronomy, Aarhus University
Ny Munkegade 120
DK-8000 Aarhus C – Denmark

Scientists in charge

Henrik Stapelfeldt
+45 871 55974
henriks@chem.au.dk

Lars Bojer Madsen
+45 871 55636
bojer@phys.au.dk

Useful Links

www.medea-horizon2020.eu
www.chem.au.dk
www.phys.au.dk
http://phd.au.dk/gradschools/scienceandtechnology

SOLIDUM PETIT IN PROFUNDIS · UNIVERSITAS ARHUSIENSIS ·

MEDEA

Molecular Electron Dynamics investigated by Intense Fields and Attosecond Pulses

This project has received funding from the European Union's **Horizon 2020** research and innovation programme under the Marie Skłodowska-Curie grant agreement No 641789.

Home institution

The node at Aarhus University comprises two departments:

Department of Chemistry

The Department of Chemistry is one of 12 departments at Science and Technology, Aarhus University. The department houses a number of the Danish National Research Foundation's Centres of Excellence, and carries out teaching tasks for many of the degree programmes at the faculty. Made up of a wide range of scientific areas, the department is expected to be a very strong partner in interdisciplinary initiatives in the future, especially regarding the Interdisciplinary Nanoscience Centre (iNANO).

The department's success is also evident in an analysis recently published by NordForsk. This study measured scientific impact by using a citation index to analyse the scientific articles published in the Nordic countries, and the Department of Chemistry was the strongest chemistry institution in the region. The citation rate was more than 50 per cent above average for Denmark and 80 per cent above the Nordic average.

The Department of Chemistry also educates the majority of chemists in Denmark, with well over 200 active BSc students, a considerable number of MSc students and more than 100 PhD students.

There are 28 permanent members of the academic staff, as well as a strong support organisation and a considerable number of affiliated researchers.

Department of Physics and Astronomy

The Department of Physics and Astronomy is one of 12 departments at Science and Technology, Aarhus University. The main objectives of the Department are to carry out research at the highest international level, to offer research based teaching at Bachelor of Science, Master of Science and PhD levels, and to exchange knowledge with other areas of society.

The Department dates back to 1933 when 'Det fysiske Institut' (the Institute of Physics) was established as a supporting institution to the medical science studies. In 1992, the Institute of Physics joined forces with the Institute of Astronomy and became the Department of Physics and Astronomy.

The Department is characterized both by its wide range of covered academic subjects and by its research at an international level. In several disciplines the Department is conducting international cutting-edge research, both in theoretical and experimental disciplines.

Group leader

Name: Henrik Stapelfeldt
Nationality: Danish
Date of birth: 1 June 1965

Short CV:

1993: PhD in Physics, Aarhus University (AU)
1994-96: Post Doc, NRC, Canada with Paul Corkum
1996-00: Assistant Professor, Dep. Chemistry, AU
2000-09: Associate Professor, Dep. Chemistry, AU
2009-: Professor, Dep. Chemistry, AU

My research includes: Manipulation and study of molecules with short laser pulses: Orientation of molecules, ultrafast chemical reaction dynamics using femtosecond time-resolved spectroscopy methods, and control of molecular conformations. The main activity is currently control and ultrafast imaging of molecules in helium nanodroplets, which is supported by an ERC advanced grant (2013-2018).

Currently my research group comprises 3 post docs, 4 PhD student, 1 master student, and 2 undergraduate students. In addition, we have an academic technician with an outstanding expertise in lasers and optics affiliated with the group.

I am involved in teaching at all levels in both physics, chemistry and optics. Also, I am the chairman of the PhD committee at the Chemistry Department.

Group leader

Name: Lars Bojer Madsen
Nationality: Danish
Date of birth: 20 November 1970

Short CV:

1998: PhD in Physics, Aarhus University (AU)
1998-00: Post Doc, MPQ, Germany, with P. Lambropoulos
2005-12: Associate Professor, Dep. Phys. and Astr., AU
2012-: Professor, Dep. Phys and Astr., AU

My research is on theory for strong-field and attosecond physics, including the time-dependent many-electron problem. The research is supported by an ERC StG (2011-16) and the Villum Kann Rasmussen Center of excellence on Quantum Scale Optical Processes (2014-2018).

Currently my research group comprises 4 post docs, and 7 PhD students.

I am involved in teaching at all levels in physics. I am the chairman of the PhD committee at the Department of Physics and Astronomy.

Offered training

Research Training Modules (RTMs)

A. Adiabatic and non-adiabatic alignment techniques (see next pages for details)

B. Introduction to Monte Carlo wave packet techniques (see next pages for details)

C. Lectures in Ultrafast Science (see Scientific Course description below for details)

Relevant Scientific Courses of the Department of Chemistry and Department of Physics and Astronomy

Ultrafast Science: *In this course the experimental advances and the accompanying theory of femtosecond and attosecond time-resolved studies are discussed, and a selection of the implications across different sub-fields of physics and chemistry is covered. (5 ECTS). See* http://kursuskatalog.au.dk/coursecatalog/Course/show/58794/	Lars Bojer Madsen Henrik Stapelfeldt Peter Balling
Experimental Optics: *The aim of the course is to provide the students with a comprehensive introduction to lasers and optics. Its main emphasis is on experimental exercises (5 ECTS). See* http://kursuskatalog.au.dk/en/coursecatalog/Course/show/58756/	Jan Thøgersen Henrik Stapelfeldt Peter Balling Michael Drewsen
Applied Laser Physics: T*oday, lasers play an important role in many technological contexts and the number of applications is ever growing. This course will cover abroad scope of applications of lasers. (5 ECTS). See* http://kursuskatalog.au.dk/en/coursecatalog/Course/show/58838/	Peter Balling Michael Drewsen
Cold Molecules*: A series of leading scientists invited from abroad will give lectures of topical areas in the field of cold molecules. (5 ECTS).*	Michael Drewsen Henrik Stapelfeldt

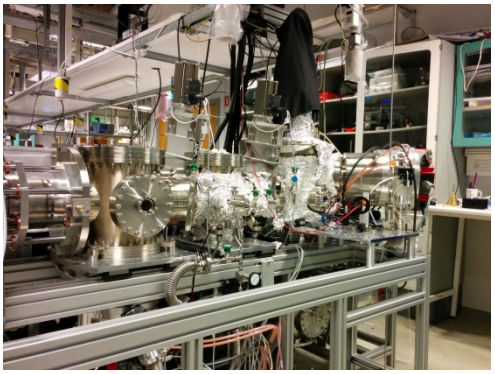
Transferable skills Modules (TSMs)

Academic English: *The goal of the course is to provide participants with the tools required and knowledge necessary, in the form of vocabulary and grammatical structures, to critique, identify and write better articles, abstracts and scientific papers*
Project Management: A Practitioner's Approach to the Managerial Process: *The objective of the course is to take a practitioners approach to project management focusing on both technical and sociocultural skills.*
Science Teaching: *The course objective is to improve your teaching skills and teaching competences as a PhD student. The course provides guidance, inspiration and tools for improving your teaching practice. During the course, you will develop and implement a teaching activity in your own teaching and use methods to provide feedback. The course addresses both traditional and online teaching and you will have the opportunity to specialise in the type of teaching which is most relevant.*
Scientific Writing and Communication: *The objective of this course is to introduce participants to the details of communication and writing scientific publications. The main emphasis is on the most common form, the "primary scientific paper", but other forms will be covered. Matters related to oral presentations, poster preparation and proposal writing will also be discussed.*
The world of research: *The course focuses on institutional, economic, political and cultural aspect of scientific research. The aim of the course is to provide PhD students with insights into interactions between science, economy, policy-making, and society.*

The transferable skills courses are offered by the Graduate School of Science and Technology, GSST, at Aarhus University and more information can be found at this link:

http://phd.au.dk/gradschools/scienceandtechnology/

A. Adiabatic and non-adiabatic alignment techniques



Objective

The goal of the RTM is to learn about laser-induced alignment of molecules in the adiabatic and non-adiabatic limit. The ESR will be involved in experiments in the Femtosecond Laser Laboratory at Aarhus University on using laser pulses to align molecules. This will involve understanding the molecular beam apparatus for the production of cold and possibly quantum-state-selected molecules, the optical beam paths for the alignment pulses and for the probe pulses, the ion spectrometer to project ions onto the 2D-detector, the detection system and the data analysis.

Equipment

The ESRs will be working with the experimental setup used for laser-induced alignment including:

Pulsed molecular valves	Supersonic molecular beams	Ultrahigh vacuum equipment	Ion detectors
CCD cameras	Acquisition software	Beam splitters	HV supplies
Beam attenuators	Nonlinear crystals	Various optical mirrors	Optical delay stages
Photodiodes	Visible spectrometer	Personal protection devices	Desktop PC

Implementation

- The training will have a series of intermediate milestones and objectives:
- Introduction to the different methods of laser-induced alignment of molecules.
- Synchronization of the alignment pulses and the probe pulses.
- Measurement of the duration of the alignment pulses.
- Preparation of the molecular sample in the pulsed molecular valve (Even Lavie)
- Recording of 2D ion images using Coulomb explosion as the probe process
- Analyzing the degree of alignment as a function of time
- Experiments with different pulse durations of the alignment pulse: Non-adiabatic versus adiabatic behavior
- Possibly alignment experiments of molecules in helium nanodroplets (if time permits)
- Analysis of data and comparison to calculations.

Duration

For the complete experiments a period of four weeks is planned. During this time the ESR will be involved mostly in the preparation of the experimental apparatus and in the data acquisition. The experiments will be conducted in collaboration and with help from local experts in the Femtolab group at AU- The completion of the RTM will also involve data analysis and numerical treatment of laser-induced alignment using newly developed software.

The period for the participation to the RTMs should be agreed upon with the host at AU.

RTM at a glance

Title	*Host institution*	*Objective*	*Duration/ Period*	*Tutors*
Adiabatic and non-adiabatic alignment	**AU**	Laser-induced alignment of molecules *experimental activity*	4 weeks / to be discussed	Benjamin Shepperson shepp@chem.au.dk Henrik Stapelfeldt henriks@chem.au.dk

B. Introduction to the Monte Carlo Wave Packet Technique

Objective

The goal of the RTM is to learn about the Monte Carlo Wave Packet technique for the description of dissociative ionization by strong near-infrared laser pulses in possible combination with attosecond pulses. The work aims at the simulation of kinetic energy release spectra for small diatomic molecules.

$$i\hbar\frac{\partial}{\partial t}|\Psi(t)\rangle = H(t)|\Psi(t)\rangle$$

Equipment

The ESRs are expected to bring their own labtops. Software and compilers for numerical implementations are available locally. In addition some sample software will be provided.

Content and implementaion

- The training will have a series of intermediate milestones and objectives::
- Introduction to dissociative ionization process
- Introduction to the Monte Carlo Wave Packet (MCWP) technique
- Simulation of radiative decay by the MCWP method
- Formulation of the dissociative ionization problem by the MCWP method
- Introduction to propagation methods for the time-dependent Schrödinger equation
- Numerical representation and propagation of the time-dependent Schrödinger equation for the hydrogen molecular ion
- Calculation of the kinetic energy release spectra for the hydrogen molecular ion

Duration

For training period of 4 weeks is planned. During this time the ESR will be guided through the content and implementation steps above.

The period for the participation to the RTMs should be agreed upon with the host at AU

RTM at a glance

Title	*Host institution*	*Objective*	*Duration/ Period*	*Tutors*
Introduction to the Monte Carlo wave packet technique	**AU**	Simulation of kinetic energy release spectra. Theory activity	4 weeks /to be discussed	Lars Bojer Madsen bojer@phys.au.dk Qingli Jing qinglijing@phys.au.dk

About the life in Aarhus

Both the Department of Chemistry and the Department of Physics and Astronomy are situated at the Aarhus Unversity campus close to the city centre. The Graduate School of Science and Technology as well as the programme committees at Department of Chemistry and Department of Physics and astronomy extensive welcome packages and information material for new PhD students.

For things to see and visit see

http://www.visitaarhus.com/ln-int/denmark/tourist-in-aarhus