

Relaxation of energized PAHs

PhD Day 2018

Gabi Wenzel

1st year PhD student

Supervisor: **Dr. Christine Joblin**

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UNIVERSITÉ
TOULOUSE III
PAUL SABATIER



Mid-Infrared Spectra

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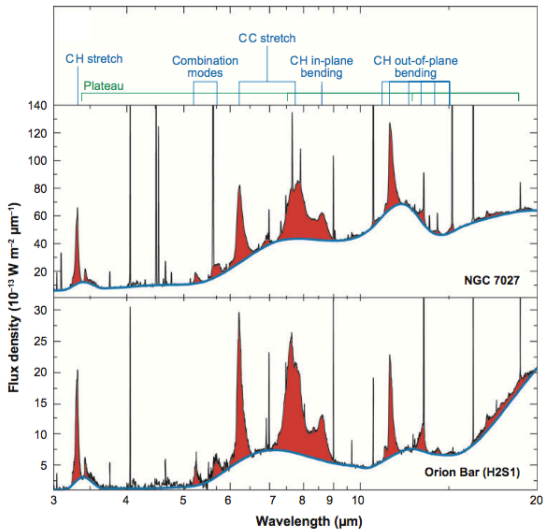
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Scientific
Context

Experimental
Methods

TD-DFT

EUROPAH



Emission features
3.3, 6.2, 7.7, 8.6,
11.2, 12.7 μm

↓
Vibrational modes of
PAHs

[1]

[1] A. G. G. M. Tielens, *Annu. Rev. Astron. Astrophys.* **46** (2008)

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Vacuum ultraviolet (VUV) photons strongly affect PAHs

Interaction of PAHs with VUV Photons

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- Absorption of VUV photons → Competing processes
 - Radiative cooling → Infrared fluorescence
 - Ionization $A^+ + h\nu \rightarrow A^{++} + e^-$
 - Fragmentation $AB^+ + h\nu \rightarrow A^+ + B$

My PhD project:

- Processes as a function of energy and molecular properties
- Photostability of PAHs in the ISM
- Ion trap experiments and mass spectrometry
- Combining experimental results with TD-DFT calculations

PIRENEA Setup at IRAP

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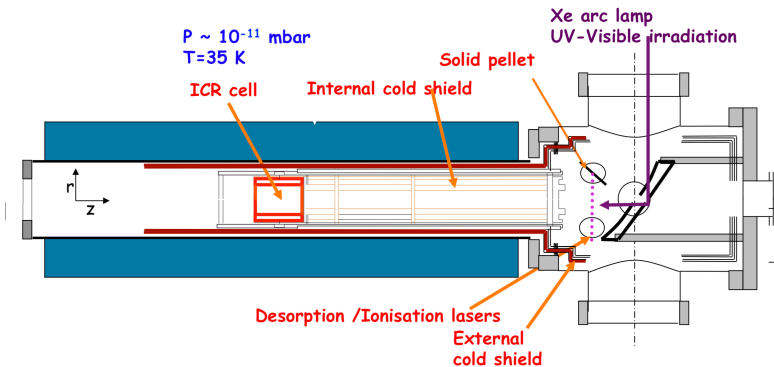
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- Piège à ions pour la Recherche et l'Etude de Nouvelles Espèces Astrochimiques



Synchrotron SOLEIL – Beamline DESIRS

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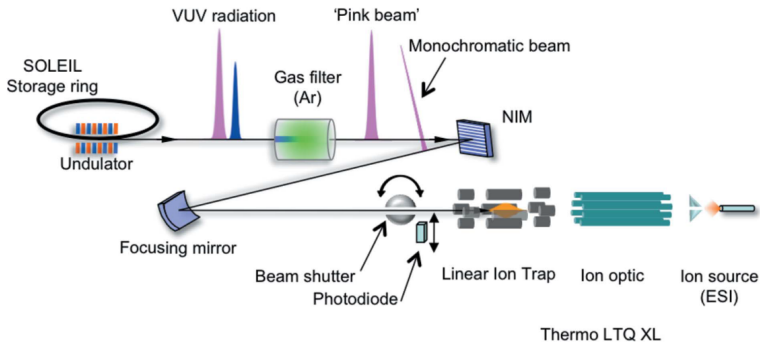
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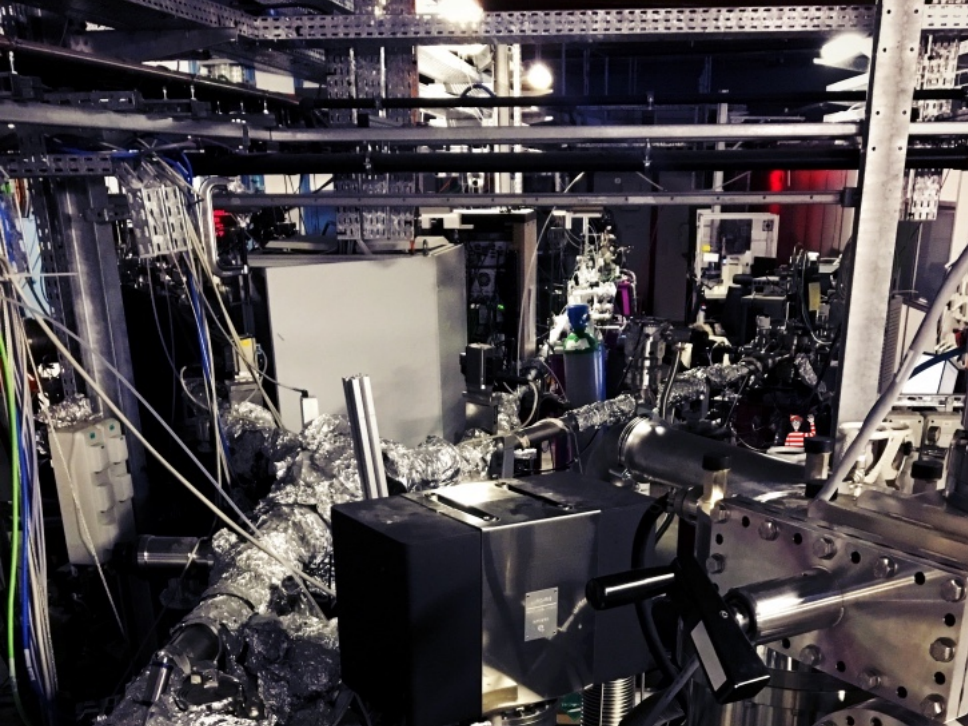
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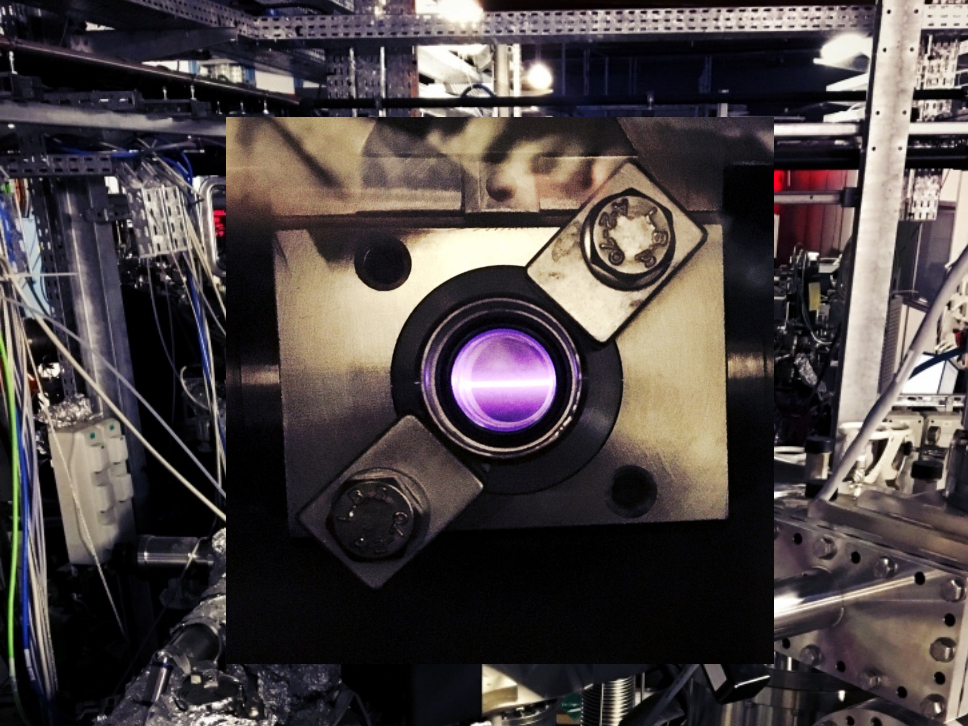
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- Tunable VUV synchrotron radiation at SOLEIL



[2] A. R. Milosavljević et al., *J. Synchrotron Rad.* **19** (2012)





Mass Spectrometry – Ionization

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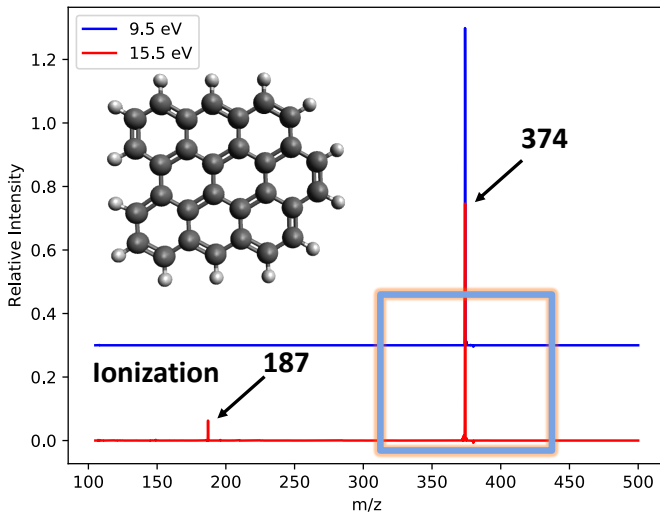
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Mass Spectrometry – Fragmentation

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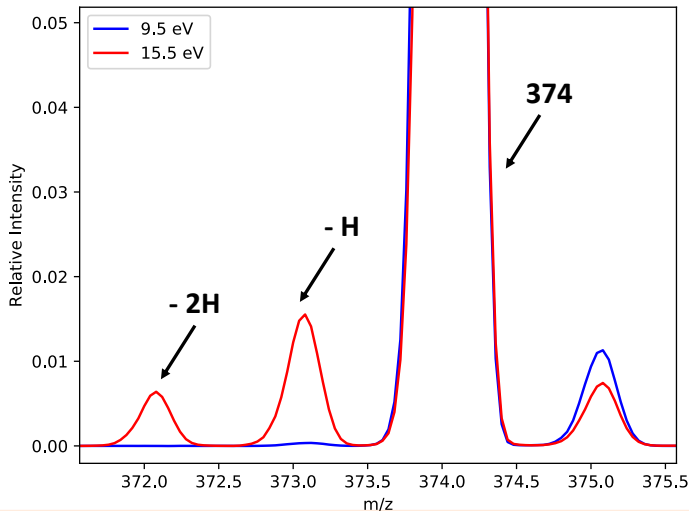
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Competition of Processes

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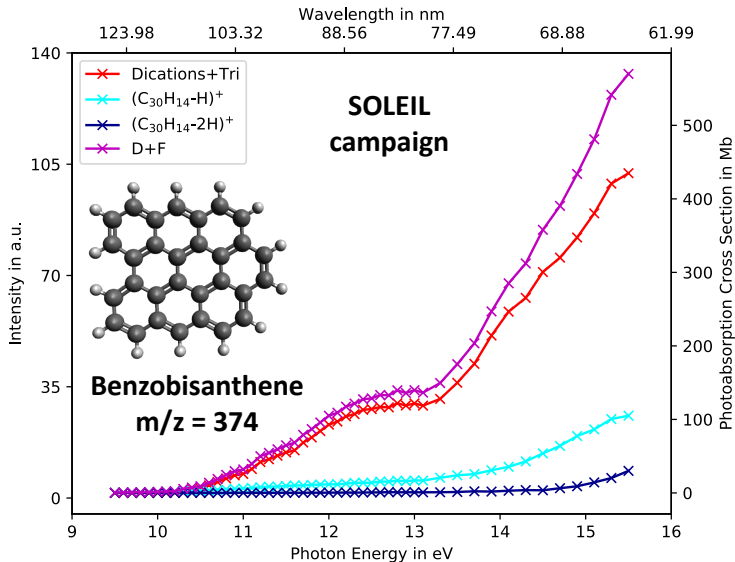
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Computed Photoabsorption Cross Section σ

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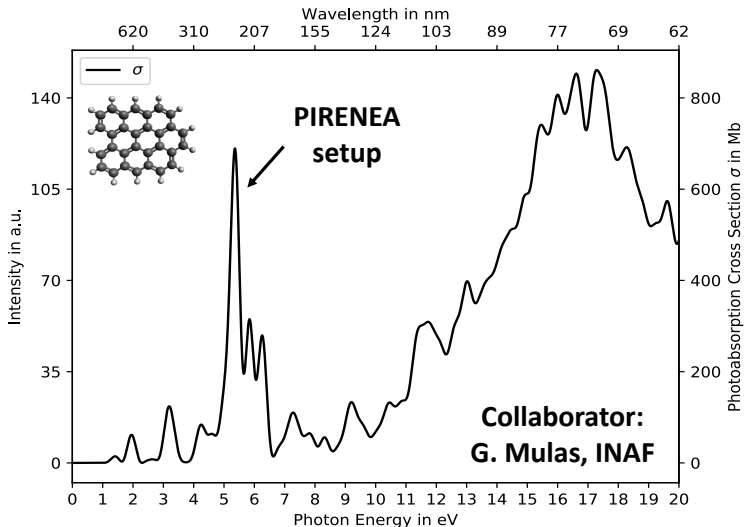
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Real space, real time implementation of TD-DFT from the OCTOPUS code

Innovative Training Network: EUROPAH

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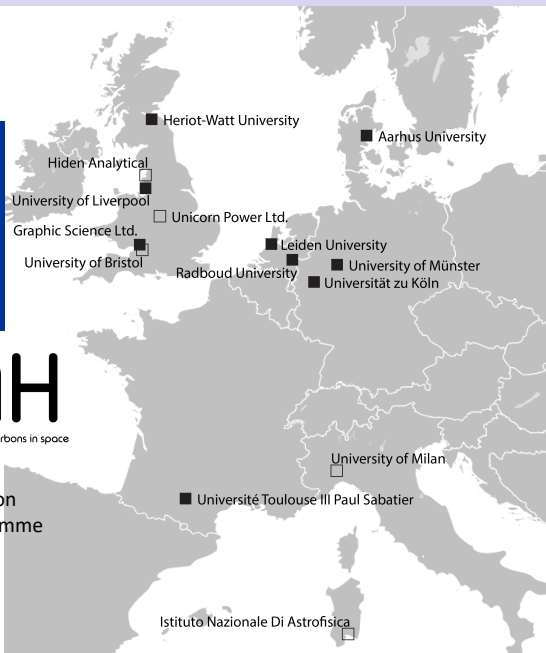
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europaH

the extensive and ubiquitous role of polycyclic aromatic hydrocarbons in space

Marie Skłodowska Curie Action
Horizon 2020 framework programme



Planned Secondment with UCO at FELion

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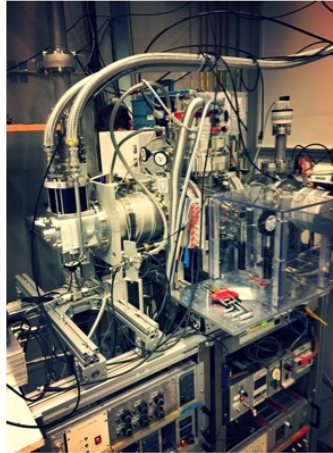
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List of Acronyms

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AES	Auger Electron Spectroscopy
AIB	Aromatic Infrared Band
DIB	Diffuse Interstellar Band
ESI	ElectroSpray Ionization
FELIX	Free Electron Laser for Infrared eXperiments
FTICR	Fourier Transform Ion Cyclotron Resonance
ISM	InterStellar Medium
KRIPES	\vec{k} -Resolved Inverse PhotoEmission Spectroscopy
LEED	Low Energy Electron Diffraction
MS	Mass Spectrometry
PAH	Polycyclic Aromatic Hydrocarbon
PES	PhotoElectron Spectroscopy
PDR	PhotoDissociation Region or Photon-Dominated Region
PIRENEA	Piège à Ions pour la Recherche et l'Étude de Nouvelles Espèces Astrochimiques
SOLEIL	Source Optimisée de Lumière d'Energie Intermédiaire du LURE*
TD-DFT	Time-Dependent Density Functional Theory
VUV	Vacuum UltraViolet
*LURE	Laboratoire d'Utilisation du Rayonnement Électromagnétique