Work Package 4:

Enhanced Understanding of the Actinide Atomic Structure

Introduction by the Work Package Leader
with support by Dag Hanstorp, UGOT Gothenburg,
Anastasia Borchevsky, RUG Groningen
Stefan Fritzsche, FSU Jena
and the respective ESR´s

LISA Mid Term Review, Nov. 25th-26th, 2020

Klaus Wendt, JGU Mainz for EU ITN LISA

This Marie Sklodowska-Curie Action (MSCA) Innovative Training Networks (ITN) receives funding from the European Union's H2020 Framework Programme under grant agreement no. 861198

Outline and Goal of the Presentation

- Meet the Request from EU side – slightly modified :

  Summary of the science covered by work package 4

  Introduction to the four ESRs

  Report on milestones and deliverables

  Report on the feasibility of achieving upcoming milestones and deliverables

→ General Presentation of the WP4 (and its present day status)

incuding the specific collaborations created for and within LISA

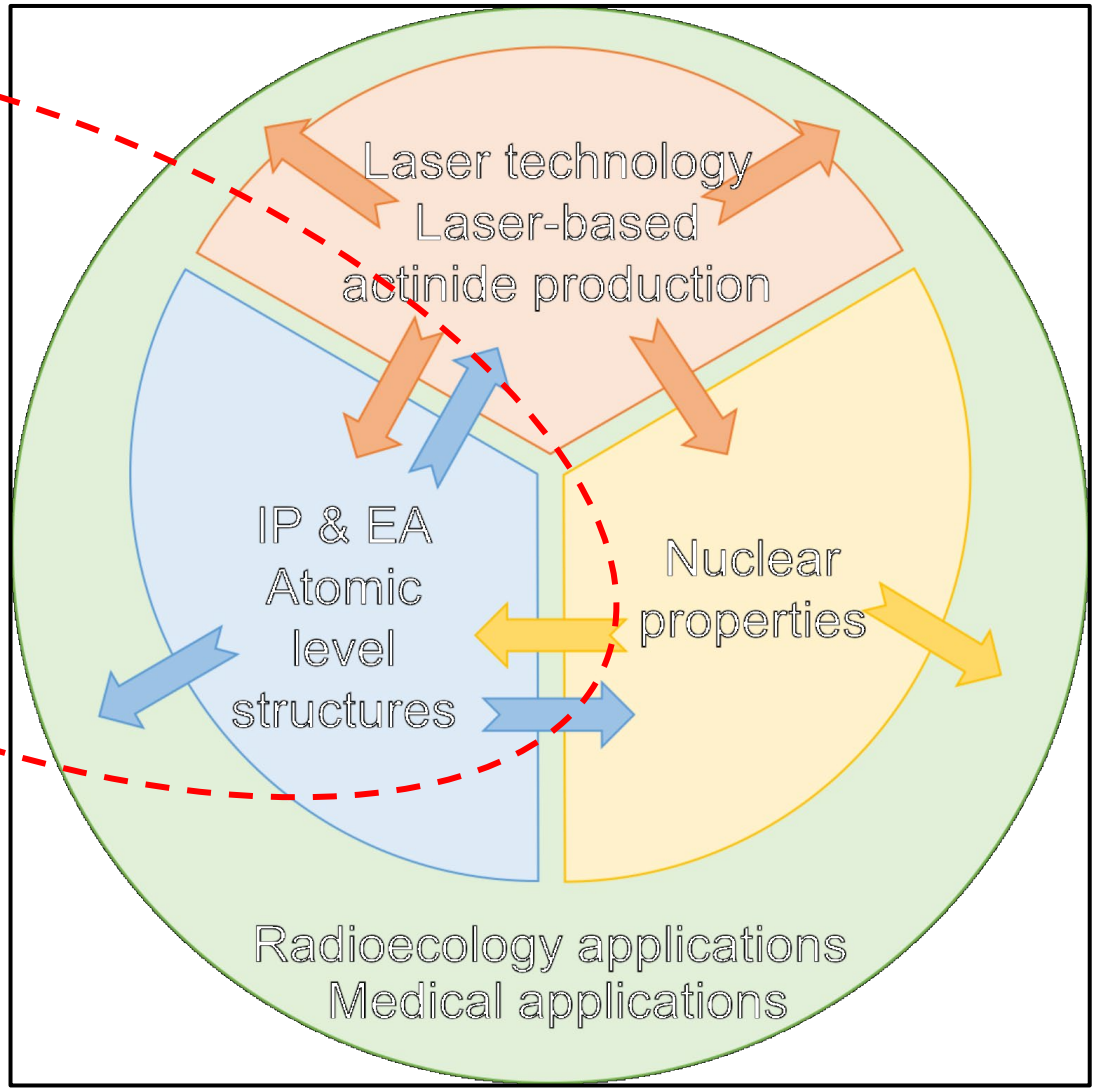
→ Turn over to individual Introduction of each WP 4 ESR

General Presentation of the WP4 Science

WP 4: Central Keystone of LISA R & D Activities

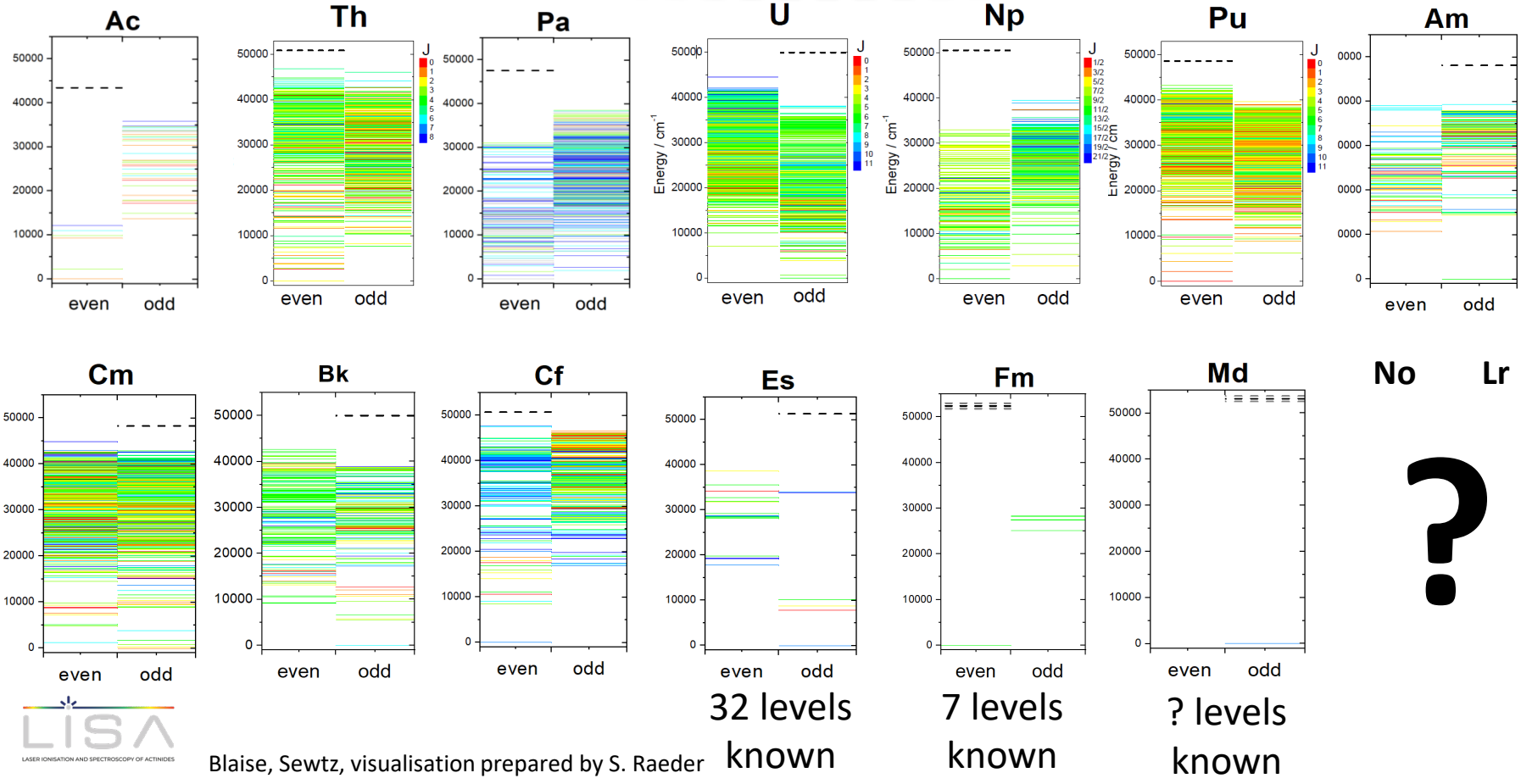
WP 4 is located specifically here

…knowledge
of the **atomic structure**
is the basis for extraction
of **nuclear properties**
& any kind of **applications**



1. Goal of WP 4: Investigate the Atomic Structure of the Actinides

Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr



LISA
LASER IONISATION AND SPECTROSCOPY OF ACTINIDES

Blaise, Sewtz, visualisation prepared by S. Raeder

Information on Actinide Atoms and Ions

- **Incomplete knowledge** of atomic level structure for **ALL** actinide (and most of the isoelectronic lanthanide) elements
- Getting increasingly **sparse** towards heavier elements
- **Hyperfine structures** only rarely known
- Ionization steps & precise value of the **ionization potential** unknown
- Existence of **stable negative ion** & value of **electron affinity** unknown
- For Z ≥ 100 (Fm) data almost exclusively only **theoretically estimated**

→ **WP 4** R & D activities on all accessible actinides as a combination of **theory** and **experiment** for atom and anion

How to access Actinide Isotopes for LISA at JGU?

Nuclear Chemistry @ JGU
operates the
TRIGA Research Reactor

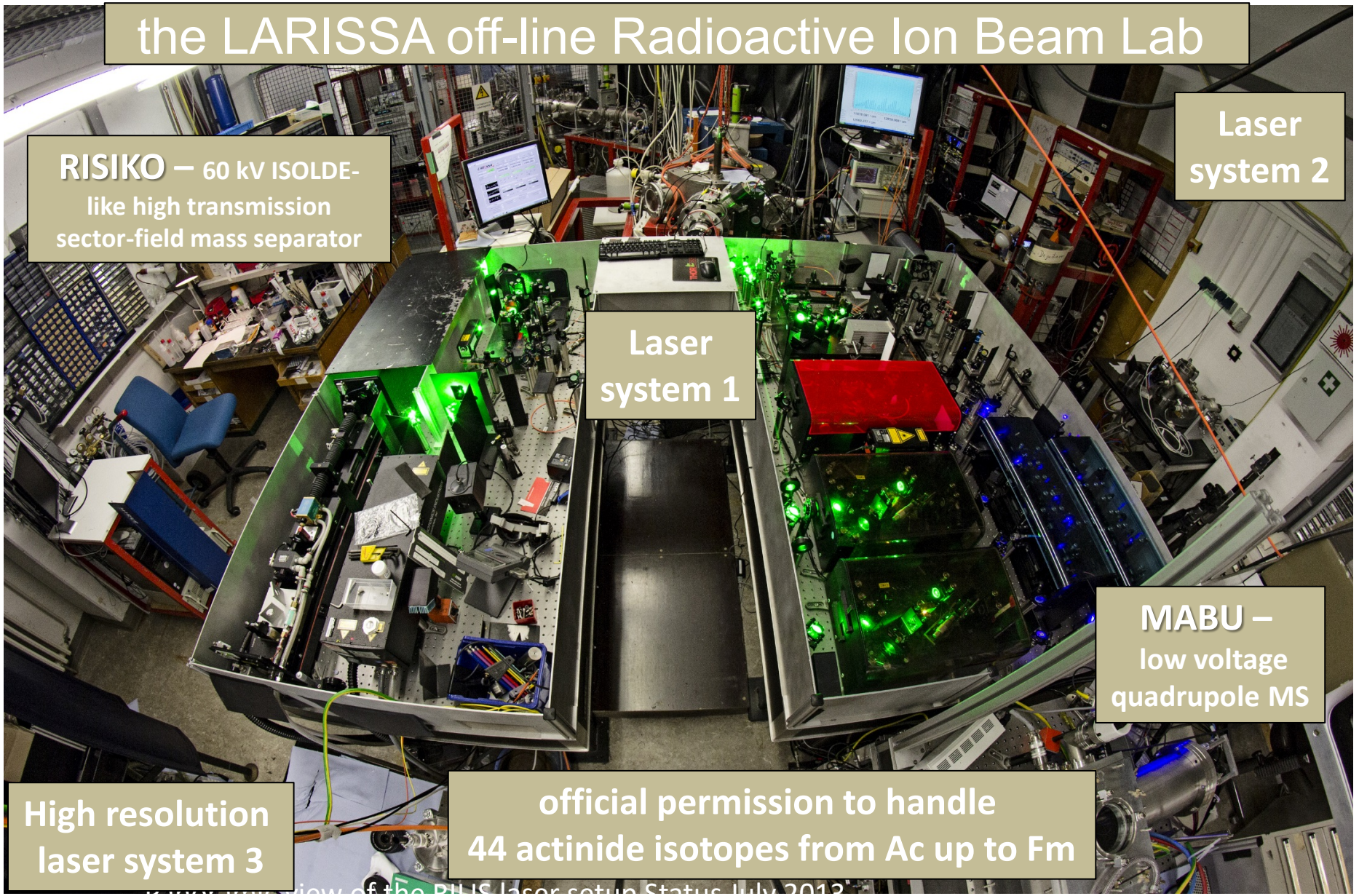
→ long lived actinide isotopes: ***on stock***

→ perfect networks and contacts towards
nuclear breeding facilities
(e.g. the high flux reactor at ORNL)
for **shorter-lived isotope** delivery
(down to few-day half-life) up to Fm

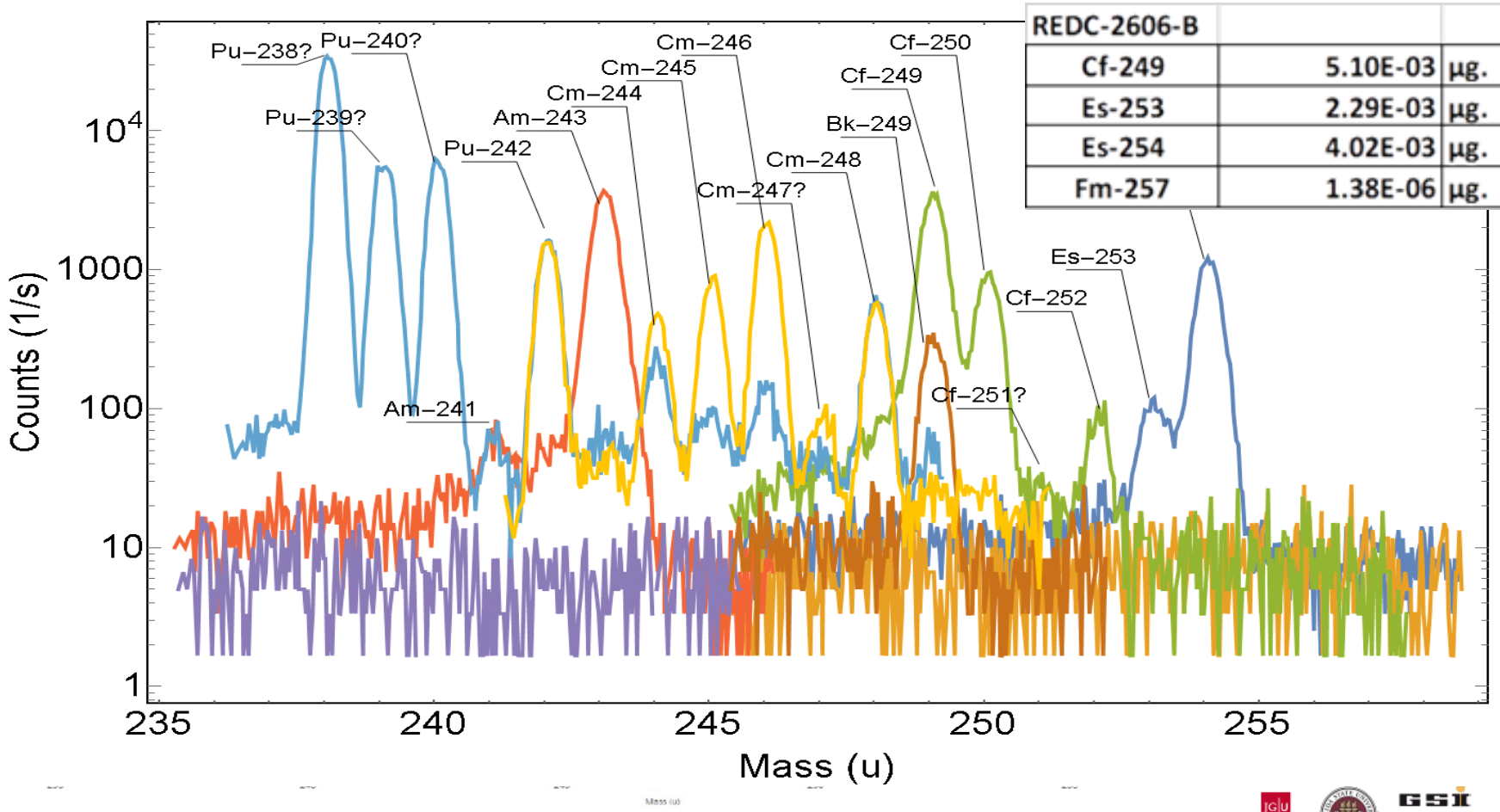
Contacts via Ch. Düllmann, D. Renisch, N. Trautmann

LISA
LASER IONISATION AND SPECTROSCOPY OF ACTINIDES

Laser Spectroscopy on Actinide atoms at JGU:



Preparatory Laser Mass Spectrometry on Actinide Mixtures



REDC-2606-B		
Cf-249	5.10E-03	µg.
Es-253	2.29E-03	µg.
Es-254	4.02E-03	µg.
Fm-257	1.38E-06	µg.

This research is supported by the U.S. DOE, Office of Science, BES Heavy Element Chemistry program. The isotopes used in this research were supplied by the U.S. DOE Isotope Program, managed by the Office of Science for Nuclear Physics.

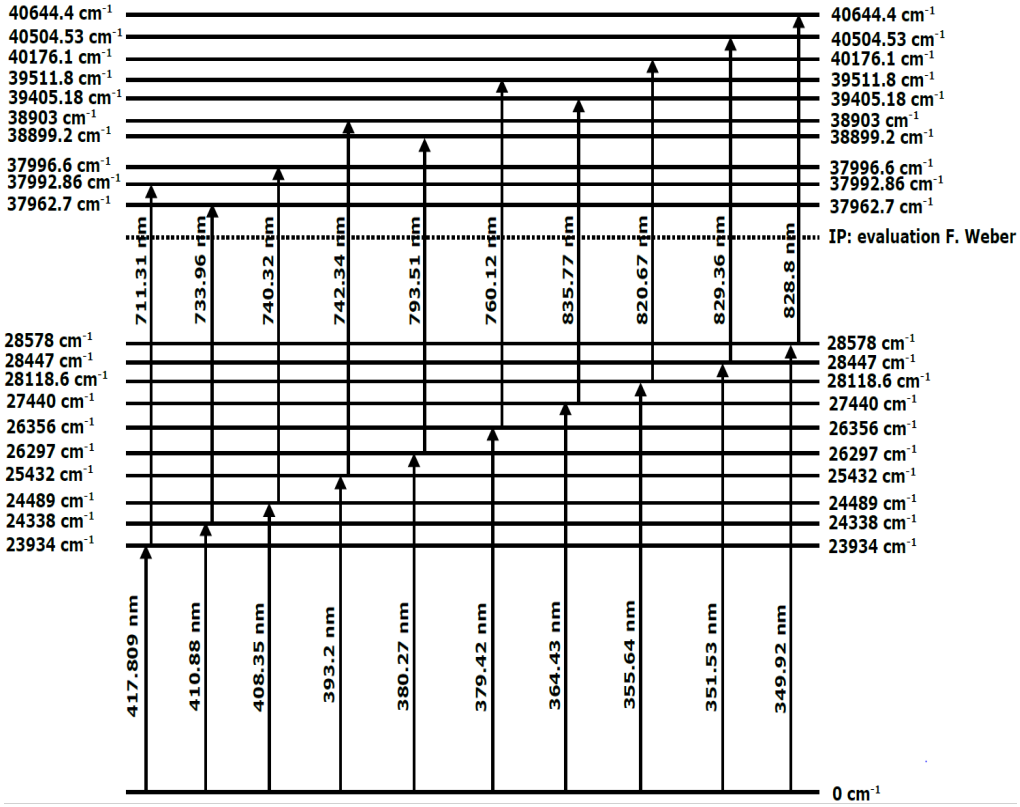
Selection of individual element by 2-step laser resonance ionization

-

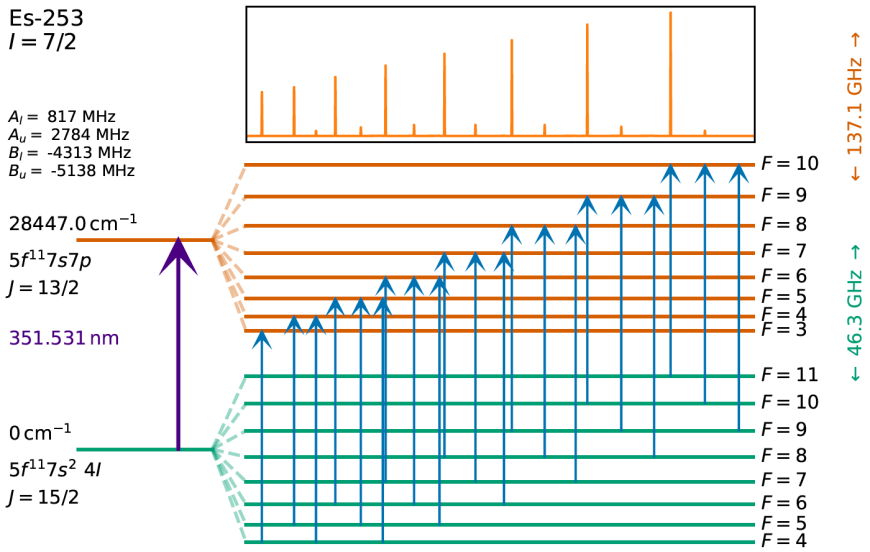
Optimum prerequisite for sensitive high resolution laser spectroscopy

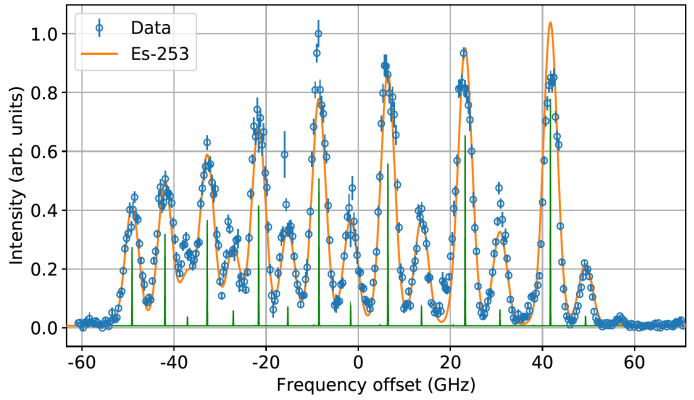
One example on one actinide isotope: ^{253}Es

^{253}Es - excitation scheme development



hyperfine structure study





Preparatory and preliminary data from 2019
to be continued and verified within LISA in 2021

LISA
LASER IONISATION AND SPECTROSCOPY OF ACTINIDES

Ionization Potentials of the Actinides by RIMS at JGU & GSI

No at GSI

Precision Measurement of the First Ionization Potential of Nobelium

P. Chhetri,1 D. Ackermann, H. Backe, **M. Block,** B. Cheal, C. Droese, Ch. E. Düllmann, J. Even, R. Ferrer, F. Giacoppo, S. Götz, F. P. Heßberger, M. Huyse, O. Kaleja, J. Khuyagbaatar, P. Kunz, M. Laatiaoui, F. Lautenschläger,1 W. Lauth, N. Lecesne, L. Lens, E. Minaya Ramirez, A. K. Mistry, S. Raeder, P. Van Duppen, Th. Walther, A. Yakushev, and Z. Zhang

Phys. Rev. Lett. 120, 263003 (2018)

11 lighter actinides At JGU

Excited atomic energy levels in protactinium by resonance ionization spectroscopy

P. Naubereit, T. Gottwald, D. Studer, and K. Wendt

Phys. Rev. A 98, 022505 (2018)

Determination of the first ionization potential of actiniumJ. Rossnagel, S. Raeder, A. Hakimi, R. Ferrer, N. Trautmann, and K. Wendt,

Phys. Rev. A 85*,1 (2012) 012525*

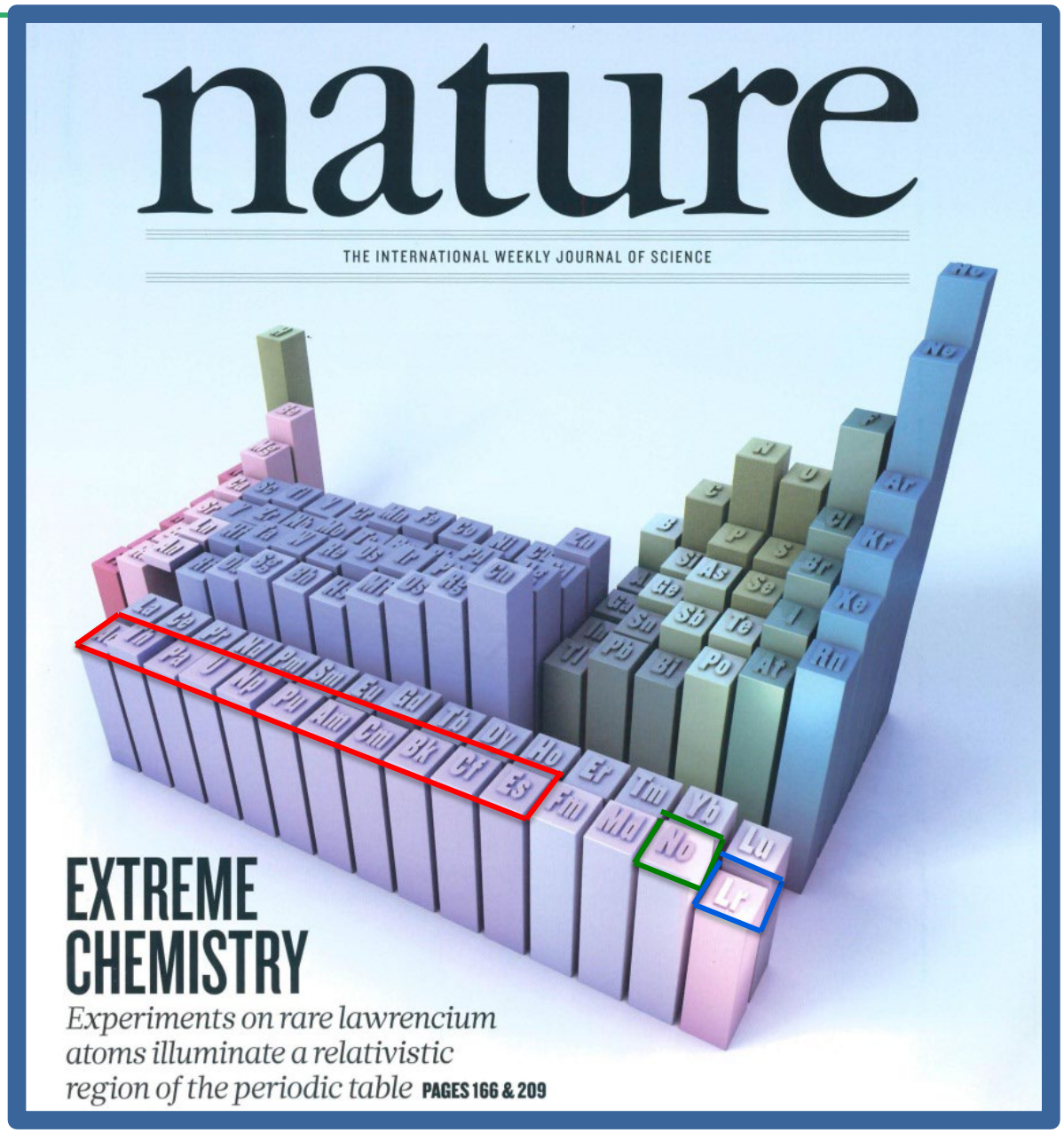
Determination of the First Ionization Potential of Actinide Elements by Resonance Ionization Mass Spectrometry

S. Köhler, R. Deißenberger, K. Eberhardt, N. Erdmann, G. Herrmann, G. Huber, J.V. Kratz, M. Nunnemann, G. Passler, P.M. Rao, J. Riegel, N. Trautmann, and K. Wendt,

Spectrochim. Acta B52*, 717-726 (1997)*

Lw at JAPAN – non laser based technique

to be verified and possibly refined within LISA



The JGU and GSI-HIM Actinide Spectroscopy Team

Sebastian Raeder

Christoph Düllmann

Mustafa Laatiaoui

Norbert Trautmann

Michael Block

KW

Experimental in WP 4

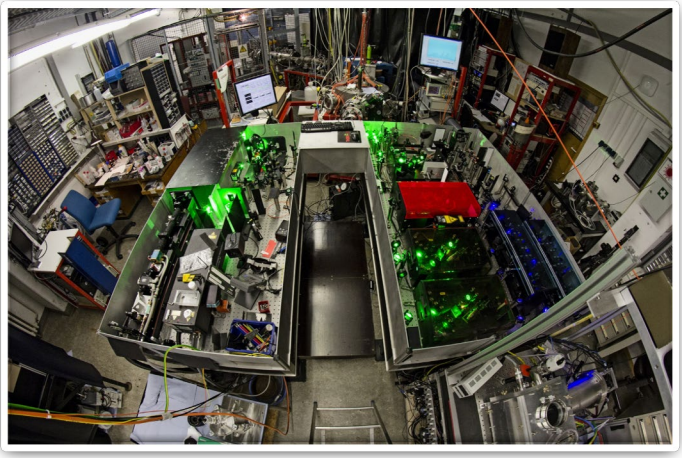
ESR 5 at JGU (Johannes Gutenberg-Universität), Mainz, Germany

PI: K.W.

ESR 5 at JGU

for the WP4 experimental package i.e. Task 1

- **JGU:** Identification of **resonance ionization schemes** for actinides using JGU Ti:Sa lasers,
  Precision (re)determination of **(IP)** of all off-line accessible actinides,
  High resolution investigation of **isotope shifts** and **hyperfine structures**
- **JYU (WP5):** expertise in actinide handling and **high resolution spectroscopy**;
- **NagoyaU: narrow linewidth laser design**; **TRIUMF:** high resolution **on-line** spectroscopy
- **FSU and RUG:** Data generation for **atomic theory** development



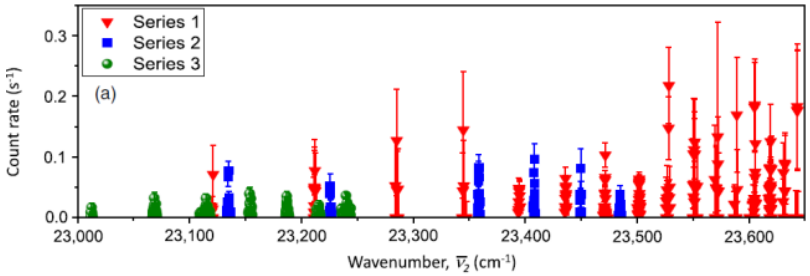
The **RISIKO** off-line laser mass separator
for actinide research & isotope purification

ERS 5: Magdalena Kaja
Started October 1st 2020

ESR 5 at JGU

within the WP4 experimental package working on Task 1

- Spectroscopy on atomic level positions and efficient excitation/ionization ladders
- High resolution investigation of hyperfine structures and isotope shifts
- Refinement and determination of ionization potentials

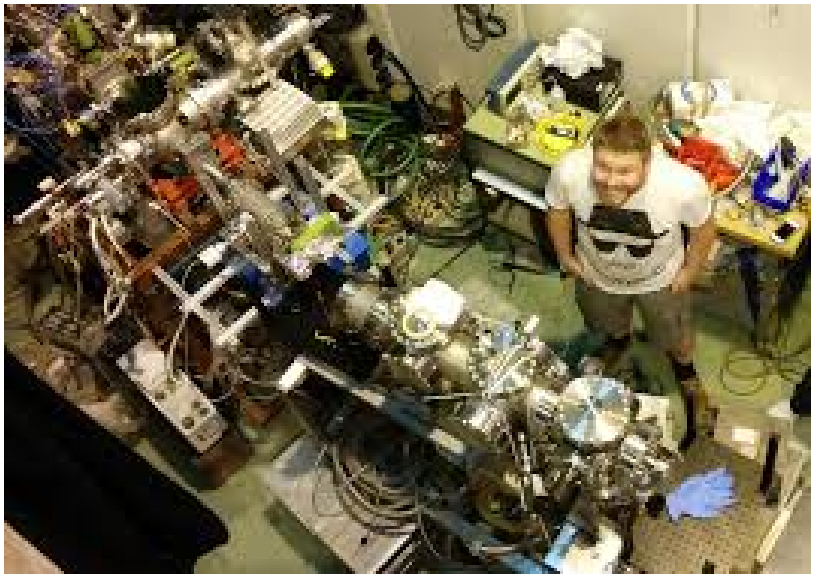


Experimental in WP 4

ESR 6 at UGOT,
Gothenburg, Sweden

PI: Dag Hanstorp

2. Goal of WP 4: Properties of Negative Actinide Ions



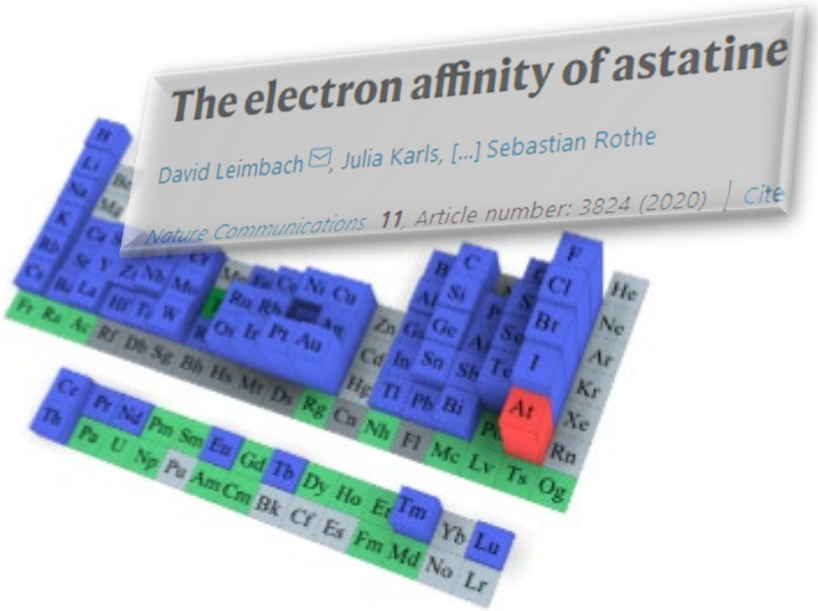
Collinear Laser Photodetachment Spectroscopy

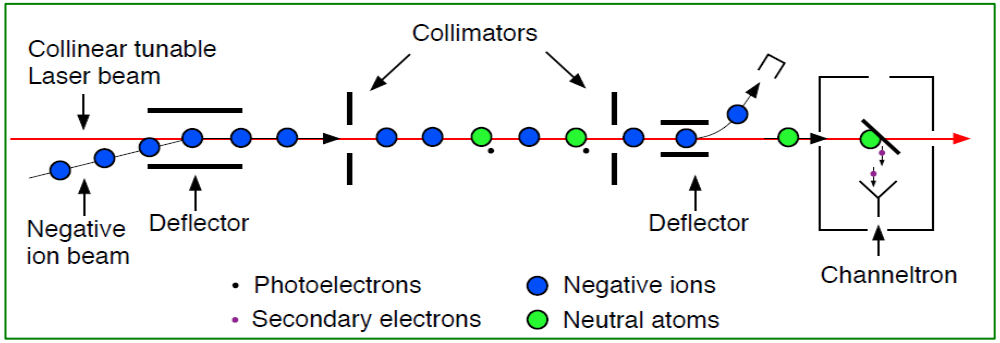
- Detachment cross section in threshold region given by the Wigner law:

$$\sigma(E) = (E_\gamma - E_{th})^{l+\frac{1}{2}}$$

- Laser photodetachment → most successful tool to determine the EA of radioisotopes

The GANDALPH facility of UGOT at ISOLDE/CERN





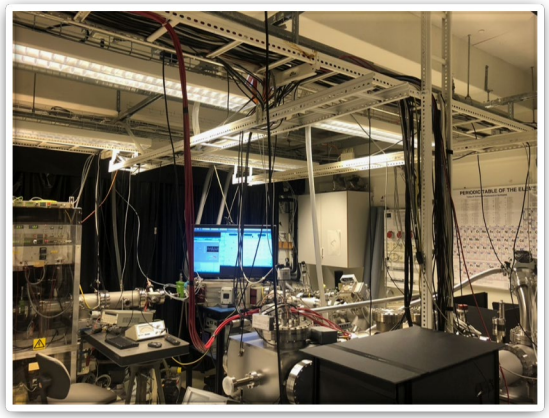
ESR 6 at UGOT

for the WP4 experimental package i.e. Task 2

- **UGOT:** Technical design of the beamline of the **GANDALPH** detector at CRIS/ISOLDE

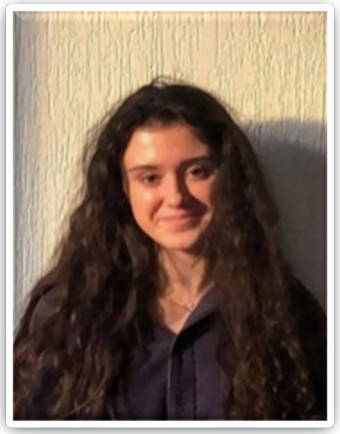
  → facilitation the determination of **electron affinities (EA)**

  using **collinear laser photodetachment spectroscopy** on negative ions
- **CERN (WP2):** production and handling of **radioisotopes**;
- **JGU: laser spectroscopy of actinides**



The GUNILLA facility in Gothenburg for studies of stable negative ions.

ERS 6: Miranda Nichols
Started Sept. 1st 2020

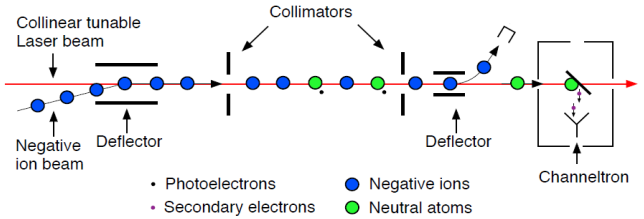


ESR 6 WP4 experimental package

→ **Electron affinities (EA) of Actinides** (& on stable isoelectronic elements)

- **Motivation:** **Negative ions** are ideal systems for tests of atomic theories beyond the **independent particles model**. For actinides also **relativistic effects** to be considered.
- **What is an EA:** The **energy** released when an electron is added to a neutral atom
- **How is it done:** Photodetachment laser spectroscopy on negative ions:

$$X^- + h\cdot\nu \rightarrow X + e^-$$



Connections to other nodes of LISA:

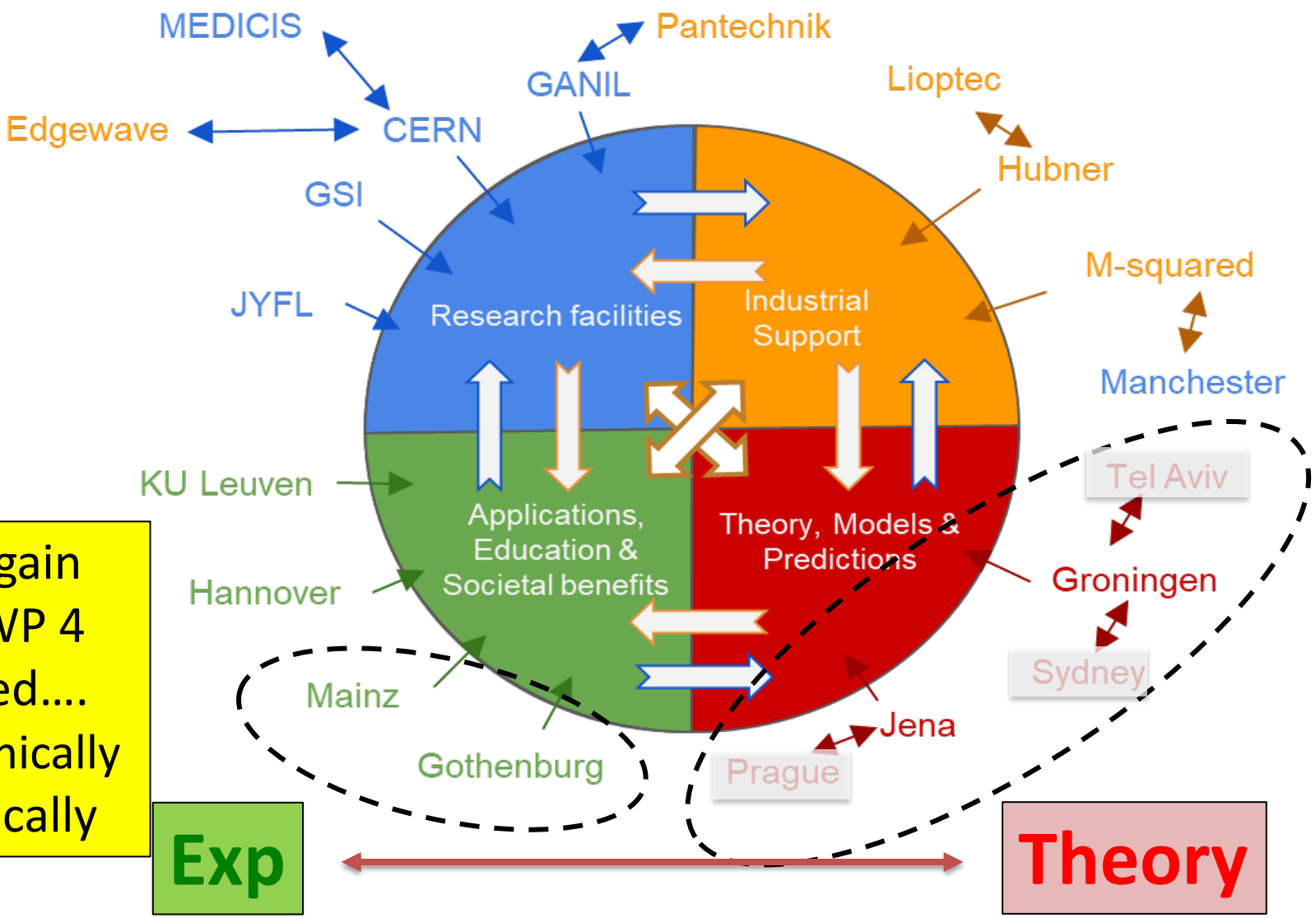
JENA and GRONINGEN: Atomic theory

ISOLDE: Production of actinides beams, negative ions spectrometer GANDALPH to be placed at CRIS/ISOLDE for EA measurements

JYVÄSKYLÄ: Experiments with GANDALPH at IGISOL

GSI: EA measurements on superheavy elements

Embedding Theory into the Experiments



This is again where WP 4 is located…. geographically and topically

THEORY in WP 4

ESR 14 at RUG (Rijksuniversiteit Groningen), the Netherlands

PI: Anastasia Borchevsky

ESR 14 at RUG

for the WP4 theory package i.e. Task 4

- **RGU:** Relativistic coupled cluster (CC) & configuration interaction (CI) atomic calculations of properties of **heavy & superheavy** elements – Program code development & application;
- **GSI & JYU** (WP5): contribution of exp. data for verification & validation;
- **TelAvivU:** development of software & calculation of quantum electrodynamics (QED)
- **USouthWales:** support & training for CI calculations

ESR 14: Raphael Crosa-Rossa
Start: August 1st 2020

LISA PhD label student
Martijn Reitsma

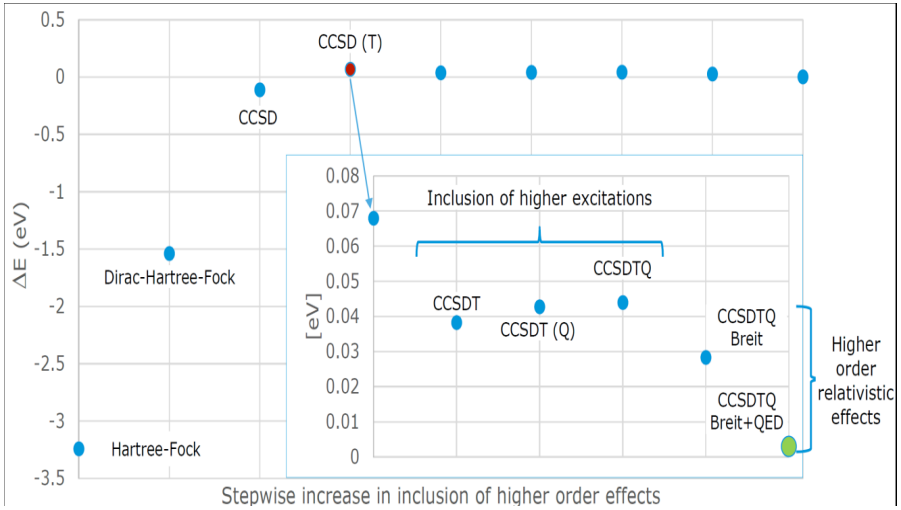
LISA
LASER IONISATION AND SPECTROSCOPY OF ACTINIDES

Theoretical support on atoms and anions

RUGroningen: Fock Space Coupled Cluster Approach limited to systems with up **to 2 valence electrons/holes** → yellow elements

High Sector Fock space coupled cluster (HSFSCC) will handle up to **4** valence electrons/holes → blue elements

University of Groningen
Groningen, Netherlands



Lanthanides	57 La	58 Ce	59 Pr	60 Nd	61 Pm	62 Sm	63 Eu	64 Gd	65 Tb	66 Dy	67 Ho	68 Er	69 Tm	70 Yb	71 Lu
Actinides	89 Ac	90 Th	91 Pa	92 U	93 Np	94 Pu	95 Am	96 Cm	97 Bk	98 Cf	99 Es	100 Fm	101 Md	102 No	103 Lr

ESR 14 WP4 theory package

→ to enhance our understanding of the actinide atomic structure

- **Raphael** will perform highly accurate **relativistic coupled cluster calculations** of the electronic structure of the elements of interest. These calculations and possible code development will be conducted within the **DIRAC** program, starting with a first project to calculate **the electron affinity of Polonium.**

- Two three-months secondments in **Tel Aviv** and **UNSW Sydney** universities are planned to get familiar with the configuration interaction (CI) approach and the Fock space coupled cluster (FSCC).

- **Martijn** has extensive experience in HFS calculations (e.g. Ge, Sn, accepted papers), **ongoing work on Bi, Sc^+,** etc..

- This will give access to the atomic properties from a theoretical perspective
  - in particular: **electronic structure, electron affinity, ionization potential or HFS**
  -
  to support as well as to give some insights in the interpretation of the experiments carried out by the others ESR within the LISA project.

Theory in WP 4

ESR 13 at FSU (Friedrich Schiller Universität), Jena, Germany

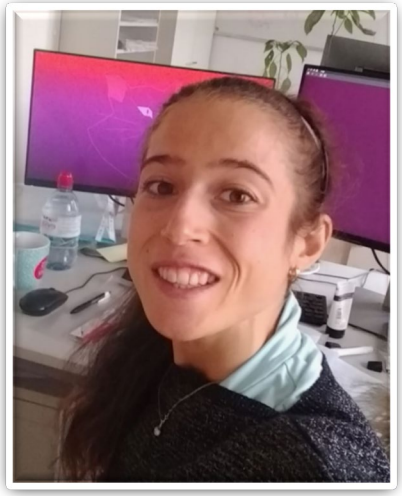
PI: Stefan Fritzsche

ESR 13 at FSU

for the WP4 theory package i.e. Task 3

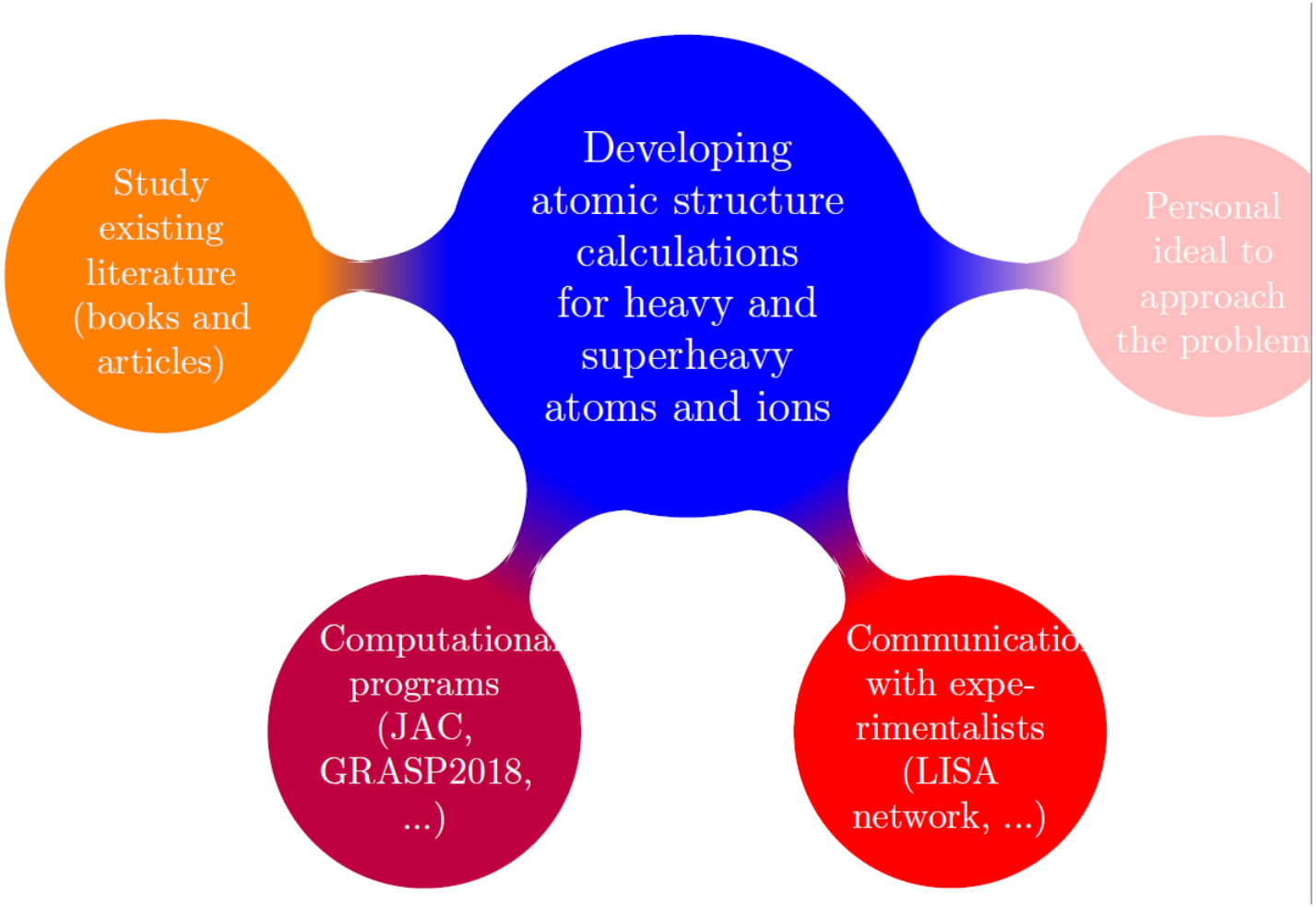
- **FSU:** Development of **dedicated atomic structure codes,** calculations for **actinide elements,** theoretical description and numerical modelling of actinide spectra;
- **RGU**: Program code **validation & testing**, development of **complementary** methods;
- **GSI & JGU** (WP5): contribution of **experimental data**, experimental **verification of data**;
- **UJK**: support and development of **parallel components for open-shell atoms**

ESR 14: Helena Escudero
Started Sept. 1st 2020



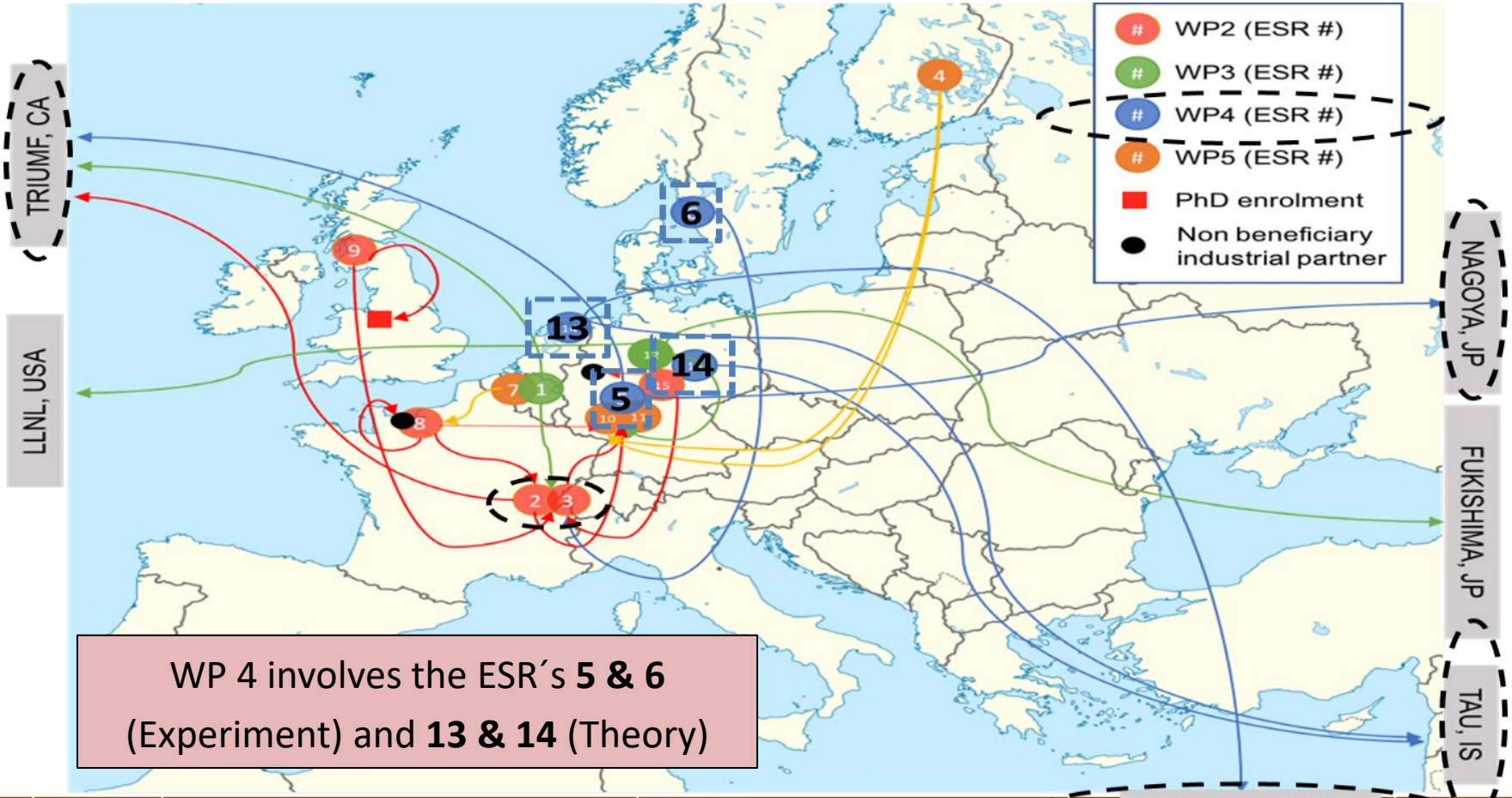
ESR 13 WP4 theory package

→ **to enhance our understanding of the actinide atomic structure further**



Status of the Recruitment, Work Activities and Secondments of the WP 4 ESRs

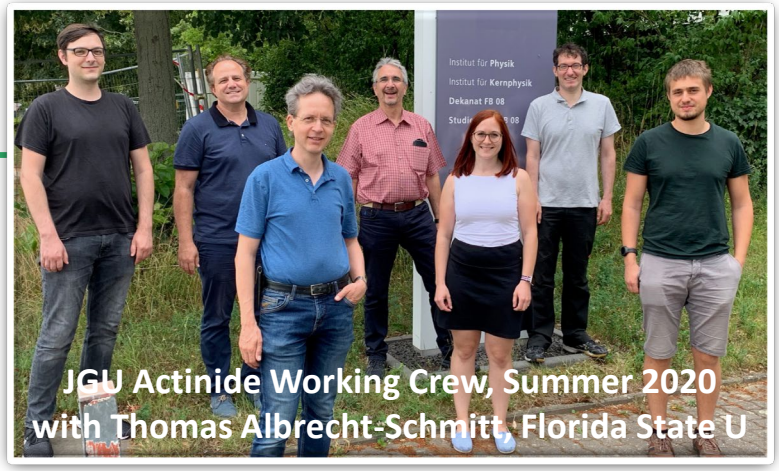
Secondments of the WP4 ESR´s - worldwide



ESR #	Host	Academic secondment	Research centre secondment	Industrial secondment	TOTAL
5	JGU	JYU M13-14; NU M17	TRIUMF M18-19	MSL M25-26	7M
6	UGOT		CERN M25-31, M38-40		10M
13	FSU	TAU M15-18; UJK M21-24			8M
14	RUG	TAU M15-18; UNSW M21-24			8M

Conclusion – WP 4 is well on its way…

…enhancing Understanding of the Actinide Atomic Structure



JGU Actinide Working Crew, Summer 2020
with Thomas Albrecht-Schmitt, Florida State U

- All four ESR´s of WP 4 recently **started**
- **initial planning** delayed by

  ≈ 2 months due to COVID-19 induced late recruitment
- WP 4 **milestones & deliverables**:

D 4.1 Calculations of properties of interest of lighter actinides by relativistic CI+MBPT method (report) [M20]

D 4.2 Application of relativistic coupled cluster & CI+MBPT approaches to superheavies (report) [M36] — theory

D 4.3 Hyperfine splitting in actinium including radiative corrections (report) [M36]

D 4.4 Basic **resonance ionization data** from Ti:Sa laser spectroscopy for 10 lighter actinides (report) [M40]

D 4.5 On-line **photodetachment** spectroscopy on actinides at ISOLDE (report) [M42] — exp

all still well ahead – seemingly feasible without significant delays