

# 10<sup>th</sup> Workshop on the Chemistry of the Heaviest Elements (CHE10)



Dunhuang, China

7 - 11 September, 2025

## Background

The CHE 10 is the tenth in the series of international workshop dedicated to recent achievements and developments in experiment and theory on the Chemistry of the Heaviest Elements. The previous series of workshops were held in Grossbothen (1991), Solothurn (1993), Mainz (1995), Stenungsund (1997), Hasliberg (2001), Oslo (2005), Mainz (2009), Takayama (2013) and Ascona (2017). The CHE10 is organized by Institute of Modern Physics, Chinese Academy of Sciences.

## Scope

This workshop will focus on the recent developments in experimental and theoretical aspects of the chemical properties of heavy actinide and transactinide elements. The scientific program will consist of invited talks and oral presentations selected on the basis of submitted abstracts.

## International Advisory Committee

Witold Nazarewicz (USA)  
Robert Eichler (Switzerland)  
Christoph E. Duellmann (Germany)  
Hiromitsu Haba (Japan)  
Sergey Dmitriev (Russia)  
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Zhiyu Sun (China)

## Local Organizing Committee

Zhi Qin  
Fangli Fan  
Yang Wang  
Shiwei Cao  
Jieru Wang

## Organizers

- The CHE10 workshop is organized by
  - Institute of Modern Physics (IMP), Chinese Academy Sciences (CAS) (中国科学院近代物理研究所).
- The CHE10 workshop is co-organized by
  - Chinese Chemical Society (中国化学会).
  - Division of Nuclear Chemistry and Radiochemistry, Chinese Nuclear Society (中国核学会核化学与放射化学分会).

## Supporters

- This workshop is supported by Bureau of International Cooperation, Chinese Academy of Sciences (中国科学院国际合作局支持).
- This workshop is supported by the National Key Research and Development Program of China (国家重点研发计划项目支持), Project No: 2024YFE0110302.

## Sponsorship

- This workshop is sponsored by Beijing Phyclover Technology Co.Ltd.

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## Online workshop materials



<https://indico.impcas.ac.cn/event/70/page/188-tips-for-che10>

## Venue

The workshop will be held in Dunhuang, Gansu, China. Dunhuang, a renowned historical and cultural city, is located in the west part of Gansu province, China. As an important part of the ancient Silk Road, Dunhuang has a history of more than 2000 years, and is known for the UNESCO World Heritage Sites, Mogao Grottoes and Crescent Moon Spring. It is a great place to implement the Global Civilization Initiative, deepen exchanges and mutual learning among civilizations.

As an important stop on the ancient Silk Road, Dunhuang once presided over the only channel from China's Central Plains to Central Asia and even to Europe. The "world's four ancient civilizations" of China, India, Greece, and Islam co-mingled there, making Dunhuang an international stage full of exotic customs and ancient legends.

Located at the westernmost end of the Hexi Corridor, Dunhuang is a county-level city in Gansu Province. Dunhuang means 'grand', and it was also called Shazhou — 'Sandy Prefecture' — historically, because the city is located at the edge of a charming desert, known as the Singing Sand Mountains.

The workshop venue is the "Dunhuang Hotel" (敦煌宾馆).

Address: 151 Yangguan middle Road, 736200 Dunhuang, China. (甘肃省敦煌市阳关中路151号, 736200).

## Some key travel tips

- Weather & Clothing

Temperature: Warm days (20 - 28 °C / 68 - 82 °F) but cooler nights (10 - 15 °C / 50 - 59 °F).

Pack: Light layers for daytime, a jacket/sweater for evenings, sunglasses, and a wide-brimmed hat for sun protection.

Footwear: Comfortable walking shoes (especially for the sand dunes and hiking).

- Sun & Desert Protection

Strong UV rays: Use high-SPF sunscreen, lip balm, and reapply often.

Dust & Wind: Bring a scarf or mask (sandstorms can occur).

Hydration: Bring drinking water — the dry climate increases the risk of dehydration.

- Cultural & Practical Tips

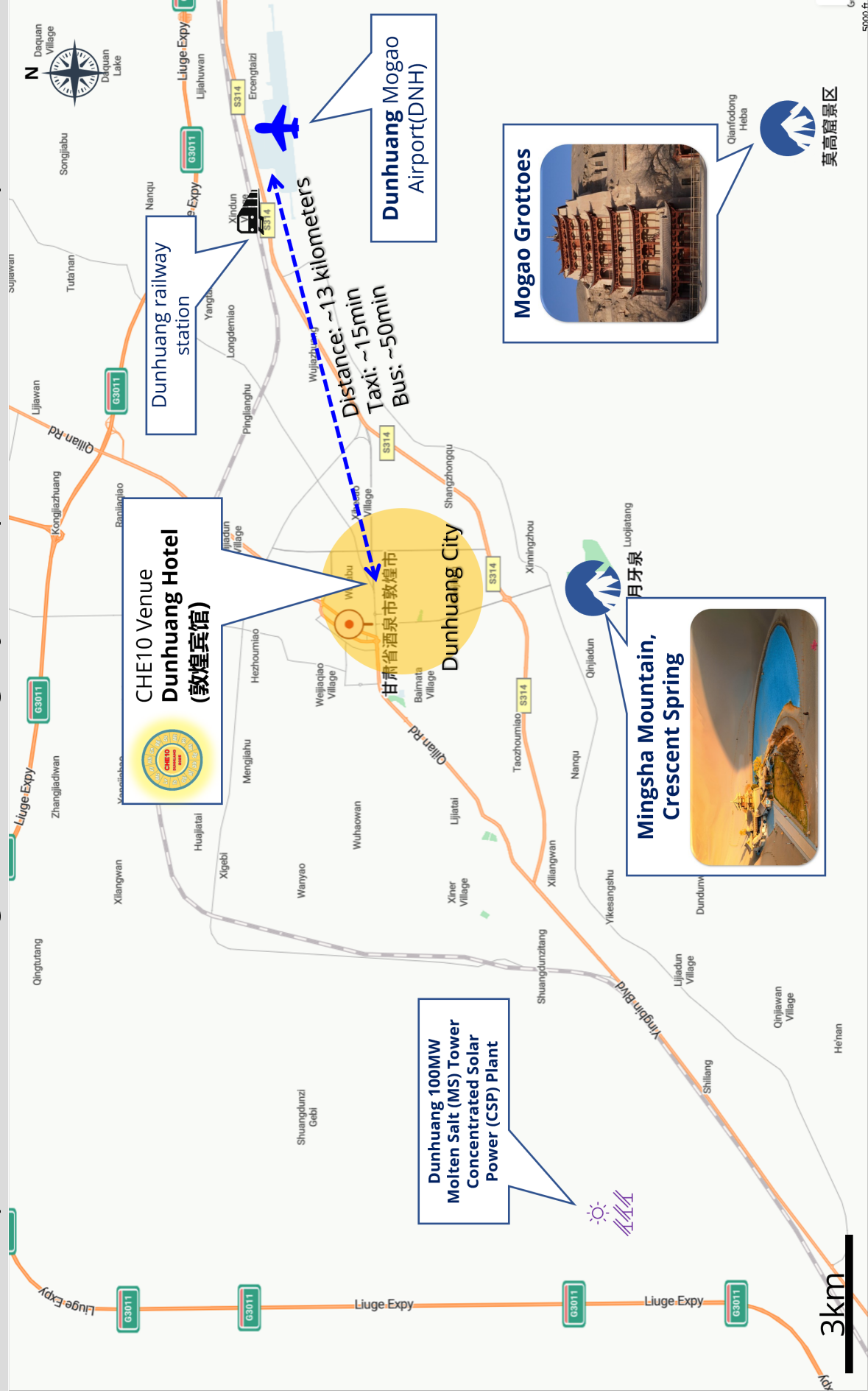
Respect local customs: No flash photography in Mogao Caves.

Cash & Payments: Some remote areas may prefer cash (though cards/WeChat Pay are widely accepted).

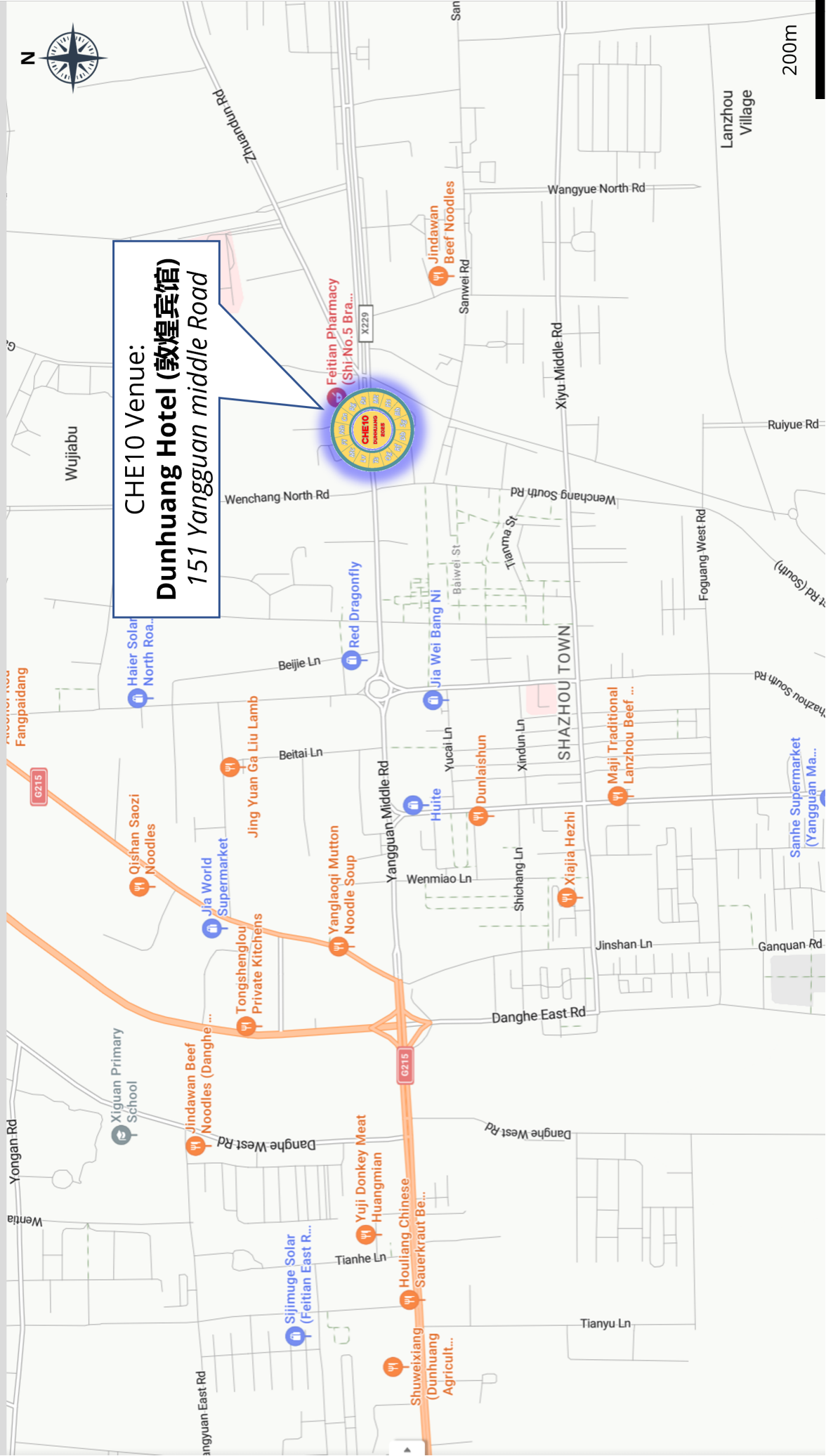
- Altitude

Dunhuang is ~1,200 m above sea level - no major altitude sickness risk, but take care to rest if sensitive.

# Map of the surroundings of Dunhuang city: Transportation and Scenic Spots



## Map around the hotel








## Program at a glance

	7 Sept 2025 (Su)	8 Sept 2025 (Mo)	9 Sept 2025 (Tu)	10 Sept 2025 (We)	11 Sept 2025 (Th)	
9:00		Opening of CHE10	Nikolay Aksenov (ID 11) *	Miroslav Iliaš (ID 12) *	Yutaka Watanabe (ID 18) *	9:00
		Meng Wang(ID 73) *	Tetsuya K. Sato (ID 57) *	Simin Wang (ID 23) *	Wenxue Huang (ID 51)	
10:00		Special Lecture: Matthias Schädel (ID 16) **	Katharina Hermainski (ID 7) *	Andrey Astakhov (ID 43)	Coffee break	10:00
		Group Photo & Coffee break	Coffee break	Coffee break	Pavel Bartl (ID 62)	
11:00		Witold Nazarewicz (ID 2) *	Fengshou Zhang (ID 9) *	Robert Eichler (ID 25)	Enni Khult (ID 17)	11:00
		Itkis Mikhail (ID 26) *	Junchen Pei (ID 39) *	Alexander Madumarov (ID 31)	Closing ceremony	
12:00		Zhi Qin (ID 59) *	Jing Su (ID 67) *	Masato Asai (ID 38)		12:00
				Yuncheng Han (ID 64)		
13:00		Lunch	Lunch	Lunch	Lunch	13:00
14:00		Weilong Chen (ID92) *				14:00
		Hiromitsu Haba (ID 24) *				
15:00		Patrick Steinegger (ID 27) *				15:00
		Coffee break	Scientific tour: Dunhuang 100MW Molten Salt (MS) Tower Concentrated Solar Power (CSP) Plant	Excursion		
16:00	Registration	Atsushi Toyoshima (ID 13) *				16:00
		Pengwei Zhao (ID 91) *				
17:00		Zhongzhou Ren (Hailan Zheng) (ID 74) *				17:00
		Zhiyuan Zhang (ID 29)*				
18:00	Reception	Banquet	Dinner	Dinner		18:00
	7 Sept 2025 (Su)	8 Sept 2025 (Mo)	9 Sept 2025 (Tu)	10 Sept 2025 (We)	11 Sept 2025 (Th)	

\*\* Special lecture (40 min); \* Invited talk (25+5 min); Oral contribution: 15+5 min.



Updated: 4 Sept. 2025

## Location


Activity	Location
 Registration	Lobby, 1F
 Workshop	Meeting room, 2F
 Reception, Lunch & Dinner	Buffet restaurant, 1F
 Banquet (Monday)	Meeting room, 2F
 Scientific tour	Bus pick-up point: the entrance of the lobby, 1F

## Program


### Sunday, 7 September 2025

Time	
09:00 - 21:00	 Registration
18:00 - 21:00	 Reception


### Monday, 8 September 2025

Time	Title & Speaker	
<i>Chair: Zhi Qin</i>		
09:00 - 09:20	Opening ceremony	20'
09:20 - 09:50	Recent progress in the Institute of Modern Physics * <b>Meng Wang, IMP CAS (ID 73)</b>	25+5'
09:50 - 10:30	In Memoriam: Prof. Dr. Jens Volker Kratz (1944-2024) ** <b>Matthias Schädel, GSI (ID 16)</b>	40'
10:30 - 11:00	 Group Photo & Coffee break	30'







Time	Title & Speaker	
<i>Chair: Yuichiro Nagame</i>		
11:00 - 11:30	Structure of Superheavy Nuclei * <b>Witold Nazarewicz</b> , <i>Michigan State University (ID 2)</i>	25+5'
11:30 - 12:00	Nuclear Reactions for synthesis SHE beyond 118 * <b>Itkis Mikhail</b> , <i>JINR (ID 26)</i>	25+5'
12:00 - 12:30	Status and Prospect of the SHE Chemistry at IMP * <b>Zhi Qin</b> , <i>IMP CAS (ID 59)</i>	25+5'
12:30 - 14:00	 Lunch	90'
<i>Chair: Witold Nazarewicz</i>		
14:00 - 14:30	China Accelerator Facility for Superheavy New Elements CAFE2 at IMP * <b>Weilong Chen</b> , <i>IMP CAS (ID 77)</i>	25+5'
14:30 - 15:00	Search for element 119 in the $^{248}\text{Cm}(^{51}\text{V}, \text{xn})^{299-x}119$ reaction * <b>Hiromitsu Haba</b> , <i>RIKEN (ID 24)</i>	25+5'
15:00 - 15:30	From gas-phase chromatography to liquid-phase experiments with superheavy elements * <b>Patrick Steinegger</b> , <i>PSI / ETHZ (ID 27)</i>	25+5'
15:30 - 16:00	 Coffee break	30'
<i>Chair: Hiromitsu Haba</i>		
16:00 - 16:30	Chemical and medical studies of astatine at the University of Osaka * <b>Atsushi Toyoshima</b> , <i>Institute for Radiation Sciences, the University of Osaka (ID 13)</i>	25+5'
16:30 - 17:00	Probing Superheavy Nuclei: Structure and Dynamics from Lattice CDFT * <b>Pengwei Zhao</b> , <i>Peking University (ID 61)</i>	25+5'
17:00 - 17:30	Calculations on alpha-decay halfives of heavy and superheavy nuclei * <b>Zhongzhou Ren (Hailan Zheng)</b> , <i>Tongji University (ID 74)</i>	25+5'
17:30 - 18:00	SHE Study at the China Accelerator Facility for Superheavy Elements * <b>Zhiyuan Zhang</b> , <i>IMP CAS (ID 29)</i>	25+5'
18:00	 Banquet	



## Monday, 9 September 2025

Time	Title & Speaker	
<b>Chair: Robert Eichler</b>		
09:00 - 09:30	Experiments on the chemistry of Cn and Fl at the focal plane of the GRAND separator * <b>Nikolay Aksenov, JINR (ID 11)</b>	25+5'
09:30 - 10:00	Chemistry of Superheavy Elements at JAEA: Current Perspectives and Developments * <b>Tetsuya K. Sato, JAEA / Ibaraki Univ. (ID 57)</b>	25+5'
10:00 - 10:30	Chemistry of SHE at GSI: from nihonium, flerovium and moscovium towards livermorium * <b>Katharina Hermainski, GSI (ID 7)</b>	25+5'
10:30 - 11:00	 Coffee break	30'
<b>Chair: Shangui Zhou</b>		
11:00 - 11:30	Some possible ways to produce superheavy nuclei * <b>Fengshou Zhang, Beijing Normal University (ID 9)</b>	25+5'
11:30 - 12:00	Theoretical issues towards synthesizing superheavy elements * <b>Junchen Pei, Peking University (ID 39)</b>	25+5'
12:00 - 12:30	Theoretical Studies of the Coordination Structures, Stabilities and Electronic Spectra of Cm <sup>3+</sup> Species at the Mineral-Water Interface * <b>Jing Su, Sichuan University (ID 67)</b>	25+5'
12:30 - 14:00	 Lunch	
14:00 - 18:00	 Scientific tour: Dunhuang 100 MW Molten Salt (MS) Tower Concentrated Solar Power (CSP) Plant	
18:00	 Dinner	

## Monday, 10 September 2025

Time	Title & Speaker	
<i>Chair: Itkis Mikhail</i>		
09:00 - 09:30	Theoretical study of adsorptions of superheavy elements and their compounds on various surfaces * <b>Miroslav Iliaš</b> , <i>BLTP JINR (ID 12)</i>	25+5'
09:30 - 10:00	Exotic decays in open quantum systems * <b>Simin Wang</b> , <i>Fudan University (ID 23)</i>	25+5'
10:00 - 10:20	Extended Monte-Carlo model for SHE adsorption simulation <b>Andrey Astakhov</b> , <i>JINR (ID 43)</i>	15+5'
10:20 - 10:50	 Coffee break	20'
<i>Chair: Nikolay Aksenov</i>		
10:50 - 11:10	Diffusion Control as part of Monte-Carlo simulation of gas chromatography <b>Robert Eichler</b> , <i>PSI / University of Bern (ID 25)</i>	15+5'
11:10 - 11:30	Upgrade of the Cryodetector setup for study the gas-phase chemistry of Cn and Fl behind the GRAND separator <b>Alexander Madumarov</b> , <i>JINR (ID 31)</i>	15+5'
11:30 - 11:50	High-resolution internal conversion electron spectroscopy for superheavy nuclei <b>Masato Asai</b> , <i>JAEA (ID 38)</i>	15+5'
11:50 - 12:10	Design and fabrication of 4H-SiC detectors for Nh study <b>Yuncheng Han</b> , <i>HFIPS CAS (ID 64)</i>	15+5'
12:10 - 14:00	 Lunch	
14:00 - 18:00	 Excursion	
18:00	 Dinner	

## Monday, 11 September 2025

Time	Title & Speaker	
<b>Chair: Xiaohong Zhou</b>		
09:00 - 09:30	Spectroscopy of neutron-rich nuclei produced by multinucleon transfer reactions * <b>Yutaka Watanabe</b> , <i>Wako Nuclear Science Center, Institute of Particle and Nuclear Physics, High Energy Accelerator Research Organization (ID 18)</i>	25+5'
09:30 - 09:50	MRTOF mass spectrometer at SHANS for fusion-evaporation residues <b>Wenxue Huang</b> , <i>IMP CAS (ID 51)</i>	15+5'
9:50 - 10:10	 Coffee break	20'
<b>Chair: Matthias Schädel</b>		
10:10 - 10:30	Liquid-phase separation systems for SHE homologs at the CTU <b>Pavel Bartl</b> , <i>CTU in Prague (ID 62)</i>	15+5'
10:30 - 10:50	Extraction behavior of fluoride complex of dubnium with tributyl phosphate <b>Masashi Murakami</b> , <i>Institute for Radiation Sciences, the University of Osaka (ID 65)</i>	15+5'
10:50 - 11:10	Nobelium Extraction from Nitric Acid with TODGA-resin <b>Enni Khult</b> , <i>The University of Osaka (ID 17)</i>	15+5'
11:10 - 11:30	Closing ceremony	
12:00	 Lunch	

\*\* Special lecture

\* Invited talk

## Book of abstracts

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**In Memoriam: Prof. Dr. Jens Volker Kratz (1944-2024)**

Matthias Schädel (GSI Helmholtzzentrum für Schwerionenforschung GmbH)

With his exceptional skills and dedication to chemistry and physics, Jens Volker Kratz was an outstanding nuclear chemist - and a friend to many of his colleagues and co-workers.

Jens Volker Kratz, born on 26 May 1944 in Jena, studied chemistry at the Johannes Gutenberg University Mainz (JGU). In 1971, he obtained his doctoral degree under the supervision of Günter Herrmann in the Institute of Nuclear Chemistry with his studies of short-lived nuclear fission products. Formative was his time with Glenn T. Seaborg (1992-74) at the Lawrence Berkeley National Laboratory (LBNL). Here, Jens participated in heavy-ion accelerator based nuclear reaction studies and the quest for superheavy elements (SHE).

Back in Germany, under Günter Herrmann's leadership as the division head and member of the board of directors, Jens played a decisive role in forming the newly established nuclear chemistry group at the GSI. He shaped the research program for a decade, which started full swing with the first U-beam from the UNILAC accelerator in 1976. In the following years, experiments were often performed in international collaboration with partners coming from laboratories in the USA, France and Switzerland, and guests from many countries including China. Together with his group, and strong support from the Institute of Nuclear Chemistry at the JGU, Jens focused on the search for SHE and on nuclear reaction studies. Aspects of the fusion of heavy nuclei, competing nucleon-transfer reactions and fission were most successfully investigated with techniques developed by the nuclear chemistry group. Jens' contribution to a deeper understanding of many of these nuclear processes were seminal.

After moving to the JGU in Mainz as a faculty member and full professor in nuclear chemistry in 1982, Jens maintained his very close ties to the nuclear chemistry group at the GSI, where many of his diploma and doctoral students performed their experiments. In the 1980s, this included series of joint experiments, first on the chemistry of heavy actinides and later on SHE, when the GSI and JGU group, together with Heinz Gägeler's group from Switzerland, did experiments, together with the LBNL group, at the 88-inch cyclotron in Berkeley. In the 1990s, experiments "returned" to GSI; many performed in large international collaborations. Unraveling chemical properties of heavy actinides and SHE in the aqueous phase, with a focus on their position in the Periodic Table of the Elements and the influence of increasingly strong relativistic effect, resulted in seminal contributions to chemistry.

At Mainz, Jens expanded his research program into related fields of atomic and nuclear physics and environmental aspects. Moreover, during his time as the dean of the faculty, he was strongly involved in the design and construction of a new building for chemistry on the campus of the JGU. Over the years, he had many administrative duties and was involved in organizational issues like founding of the Helmholtz Institute Mainz.

After his retirement in 2009, Jens kept close contact to all science aspects he was interested in. Most important for him was his last opus. Most diligently, he worked writing the Fourth Edition of the textbook "Nuclear and Radiochemistry" ; published by Wiley-VCH, 2022.

My contribution will focus on early searches for SHE, selected experiments on the chemistry of the heaviest elements and some facets of nuclear reaction studies. In between, I will briefly touch fond and personal memories of Jens Volker Kratz, a friend for decades.

## Structure of Superheavy Nuclei

Witold Nazarewicz

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The Periodic Table is still growing. In 2016, four new elements were added: nihonium, moscovium, tennessine, and oganesson. These elements define the current upper limits of mass and atomic numbers. As such, they carry the potential to transform the way we currently understand nuclear and atomic physics, and chemistry.

All superheavy nuclei are part of a vast, totally unknown region of the nuclear landscape that scientists are trying to uncover. Questions motivating the search for these systems include: What are the heaviest nuclei and atoms that can exist? Are superheavy systems different from lighter nuclear species? Is there an island of very long-lived nuclei? How can superheavy nuclei be produced? Questions such as these provide formidable challenges for both experiment and theory. This talk will review recent theoretical progress in this field of research.



## Implementation of the JINR SHE Factory program

Sergey N.Dmitriev, Vladimir K.Utyonkov, Yuri Ts.Oganessian

Flerov Laboratory of Nuclear Reactions, JINR, Dubna, Moscow reg., Russia

The discovery of a new area (island) of stability and the very fact of the existence of superheavy elements with  $Z = 112-118$  raised a number of new questions related to the fundamental properties of nuclear matter: whether even heavier nuclei can exist, whether the “Island of stability of SHE” is the last on the chart of nuclides, whether superheavy nuclei can be formed in the processes of nucleosynthesis (SHE in nature), whether D.I. Mendeleev’s Periodic Law is observed in the region of SHE.

The search for answers to these questions is the main goal of the SHE Factory created at JINR, which includes a DC280 cyclotron (with an intensity of medium-energy heavy ion beams an order of magnitude higher than previously achieved) and new high-efficiency and low-background separators. Already in the first experiments performed at the Factory on the synthesis of elements 114 and 115, the previously obtained results were not only fully confirmed, but also new isotopes of SHE ( $^{264}\text{Lr}$ ,  $^{268}\text{Sg}$ ,  $^{272}\text{Hs}$ ,  $^{275,276}\text{Ds}$ ,  $^{280}\text{Cn}$ ,  $^{286}\text{Mc}$ ,  $^{288,289}\text{Lv}$ ) were discovered.

Currently, together with the institutes of the Russian Academy of Sciences and ROSATOM RF, a project is being implemented to synthesize the first elements of the 8th period with  $Z = 119, 120$  in the reactions  $^{249}\text{Bk}$  and  $^{249}\text{Cf}$  with  $^{50}\text{Ti}$ , a separator for studying the properties of SHE with lifetimes  $\geq 30$  ms and a time-of-flight mass analyzer with  $\Delta M/M = 10^{-7}$  are created, as well as a wide program of experiments is planned.

## Status and Prospect of the SHE Chemistry at IMP

Z. Qin<sup>1\*</sup>, Y. Wang<sup>1</sup>, S.W. Cao<sup>1</sup>, X.J. Yin<sup>1</sup>, Z.M. Jia<sup>1</sup>, Y.F. Cui<sup>1</sup>

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Due to the extremely low production yield and short half-lives, experiments to explore the chemical properties of SHEs (superheavy elements,  $Z > 103$ ) always rely on state-of-the-art equipment. IMP (Institute of Modern Physics, Chinese Academy of Sciences) has successfully commissioned the China Accelerator Facility for superheavy Elements (CAFE2) and the gas-filled recoil separator SHANS2<sup>1</sup>, which offer us the opportunity to perform experiments on the chemistry of SHEs in China.

Recently, a thermochromatography detection system named LEGEND (on-Line Experiment in Gas-phase for Nihonium Detector) has been developed in IMP for the chemical study of SHEs<sup>2</sup>. On-line test experiments with short-lived Fr and Tl isotopes have been performed. Rotating <sup>243</sup>Am targets with a diameter of 20 cm were successfully prepared. First exploration with a <sup>48</sup>Ca beam and <sup>243</sup>Am targets at CAFE2 and SHANS2 was performed using the LEGEND with high performance 4H-SiC detectors<sup>3</sup>, and one <sup>288</sup>Mc ( $Z = 115$ ) event was observed at the high temperature zone (65°C) on a Si<sub>3</sub>N<sub>4</sub> surface. <sup>266</sup>Bh ( $Z = 107$ ) is also available in the <sup>243</sup>Am(<sup>26</sup>Mg,3n) reaction at CAFE2 and SHANS2. Based on the above achievements, experimental study on the chemistry of Nh ( $Z = 113$ ) and Mc, as well as the Bh carbonyls will be carried out at IMP in the near future.

## Search for element 119 in the $^{248}\text{Cm}(^{51}\text{V},\text{xn})^{299-\text{x}}119$ reaction

Hiromitsu Haba (RIKEN)

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Status of the new element search project at RIKEN is presented. In April 2018, we formed the new SHE Research Group (nSHE RG) and started an experiment to synthesize new element 119 in the  $^{248}\text{Cm}(^{51}\text{V},\text{xn})^{299-\text{x}}119$  reaction using GAs-filled Recoil Ion Separator II (GARIS-II) at RIKEN Ring Cyclotron<sup>1</sup>. The  $^{248}\text{Cm}$  target material was supplied from Oak Ridge National Laboratory. In January 2020, RIKEN heavy-ion Linear ACcelerator (RILAC) was upgraded with the 28-GHz superconducting ECR ion source and the superconducting RILAC (SRILAC). We developed the new separator GARIS-III at SRILAC. An optimal reaction energy in the  $^{248}\text{Cm} + ^{51}\text{V}$  fusion reaction was deduced from the quasielastic barrier distribution extracted by measuring the excitation function of quasielastic backscattering<sup>2-4</sup>. Since October 2020, we have continued the synthesis experiment of element 119 with GARIS-III at SRILAC.

### References

- <sup>1</sup> H. Sakai et al., Eur. Phys. J. A 58, 238 (2022).
- <sup>2</sup> T. Tanaka et al., Phys. Rev. Lett. 124, 052502 (2020).
- <sup>3</sup> M. Tanaka et al., J. Phys. Soc. Jpn. 91, 084201 (2022).
- <sup>4</sup> P. Brionnet et al., Phys. Rev. C 110, 064601 (2024).

## From gas-phase chromatography to liquid-phase experiments with superheavy elements

Patrick Steinegger

Paul Scherrer Institute / ETHZ

Gas-adsorption chromatography has been successfully used to study the adsorption behavior of superheavy elements (SHEs) on various stationary phases. To this day, it remains one of the most efficient methods for studying the chemical properties of the heaviest elements and their compounds at the one-atom-at-a-time level. However, the inherent difficulty of such experiments relates to the chemical speciation, which cannot be easily determined. Moreover, current SHEs under investigation, such as nihonium (Nh,  $Z = 113$ ), are more chemically reactive than (quasi-)closed-shell elements such as copernicium (Cn,  $Z = 112$ ) and flerovium (Fl,  $Z = 114$ ). Studies of the heaviest elements in the periodic table are further complicated by the fact that the half-lives of known isotopes of SHEs beyond flerovium drop into the millisecond range. Meanwhile, meitnerium (Mt,  $Z = 109$ ), darmstadtium (Ds,  $Z = 110$ ), and roentgenium (Rg,  $Z = 111$ ) have thus far managed to avoid chemical characterization entirely.

Therefore, there is a clear need to improve existing gas chromatography techniques and develop new experimental approaches to address the aforementioned challenges. Here, we discuss the inherent difficulties and limitations of gas-adsorption chromatography experiments in the continuum flow regime when studying more chemically reactive SHEs, such as Nh. This is exemplified by detailed on- and off-line experiments with Tl as the lighter homolog of Nh. Next, we present the progress made with vacuum adsorption chromatography using millisecond short-lived radioisotopes of the lighter homologs under conditions that are otherwise identical to those in SHE experiments. Lastly, we briefly discuss new avenues for electrochemical experiments with SHEs.

### Co-authors:

Co-authors will be mentioned in the individual parts during the presentation.

## Chemical and medical studies of astatine at the University of Osaka

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At the University of Osaka, we began a collaborative project in nuclear medicine approximately ten years ago, using a short-lived radioisotope astatine-211 ( $^{211}\text{At}$ ) which has a half-life of 7.2 hours. Targeted alpha therapy (TAT) using alpha-emitters has attracted significant attention worldwide due to its high therapeutic efficacy against cancer. Internationally, research and development in TAT has primarily focused on actinium-225 ( $^{225}\text{Ac}$ ) with a 10-days half-life. However, in Japan, regulatory constraints make the use of its target material, thorium-232 ( $^{232}\text{Th}$ ), in nuclear spallation particularly challenging. Consequently, we have focused on  $^{211}\text{At}$ , which is produced in the  $^{209}\text{Bi}(\alpha, 2n)^{211}\text{At}$  reaction. Our group has been responsible for the production of  $^{211}\text{At}$  at the AVF cyclotron facility in our university and its chemical separation by dry distillation. To date, we have successfully achieved the quantitative supply of  $^{211}\text{At}$  in aqueous solution. After developing radiopharmaceuticals using  $^{211}\text{At}$ , clinical trials for thyroid and prostate cancers were eventually initiated in the University of Osaka Hospital. In parallel with the medical application, we also carry out fundamental chemical studies of At in both gas and aqueous phases. In this presentation, we will provide an overview of TAT using  $^{211}\text{At}$  at the University of Osaka, and particularly on our investigation of halogen bonding in At compounds by gas chromatography.

## SHE Study at the China Accelerator Facility for Superheavy Elements

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The state-of-the-art China Accelerator Facility for Superheavy Elements (CAFE2) has been successfully commissioned for studies of heavy and superheavy nuclei since its full operational deployment in early 2022. During its commissioning phase, a newly constructed gas-filled recoil separator, SHANS2, demonstrated breakthrough capabilities with high transmission efficiency and background suppression through a series of test reactions.

Several reactions dedicated for the discovery of new isotopes and the spectroscopy studies on SHE were carried out at the setup. In this talk, we will present the recent status of CAFE2 and the performance of SHANS2. The results about the new neutron-deficient isotopes,  $^{203,204}\text{Ac}$ ,  $^{210}\text{Pa}$ , and the spectroscopy studies on  $^{261,262}\text{Bh}$  and  $^{247}\text{Md}$  will be reported as well, which demonstrate the tremendous capability of the facility for the study of heavy and superheavy nuclei.

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## Experiments on the chemistry of Cn and Fl at the focal plane of the GRAND separator

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The chemistry of Cn and Fl has been the subject of long-term studies by two collaborations, which formed scientific chemistry programs at the accelerator laboratories FLNR and GSI<sup>1,2</sup>. Despite the obtained outstanding results, both experimental series are not conclusive due to the unpredicted observation of two adsorption zones in gas thermochromatography. The small number of observed Fl atoms also introduces an element of uncertainty in the interpretations of this observation. In the first series of experiments at the SHE Factory, before further detailed speciation studies, we repeat the TASCA experiment with the Dubna improved chemical setup behind the GRAND separator. Experiments on the synthesis of <sup>286,287</sup>Fl in the reaction <sup>242</sup>Pu(<sup>48</sup>Ca,3-4n) using the DGFRS-2 and GRAND separators were preceded chemical studies<sup>3,4</sup>. The setup called Cryodetector, previously used for Nh studies<sup>5</sup>, was equipped with a new RTC designed for the focal plane of the GRAND separator. New gold coated detectors array with and an extended temperature gradient down to -170 °C were fabricated. In the ongoing experiments, 8 decay chains assigned to adsorption of <sup>287</sup>Fl and <sup>283</sup>Cn were detected indicating two deposition zones at room temperature and around -100 °C, confirming previous observations.

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## CURRENT STATUS AND FUTURE PERSPECTIVES OF SUPERHEAVY ELEMENT CHEMISTRY AND HEAVY ELEMENT SCIENCE AT JAEA

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Studying the chemical properties of superheavy elements (SHEs) and heavy actinides provides valuable insights into the impact of relativistic effects on their chemical properties. The large nuclear charge of these elements can lead to strong relativistic effects, which might cause their chemical behavior to deviate from established periodic trends. However, significant challenges arise in conducting experiments due to the short half-lives and low production rates, which often limit them to generating just one atom at a time.

At the Japan Atomic Energy Agency (JAEA), we are tackling these challenges by employing rapid radiochemical techniques and an isotope separator on-line (ISOL) system. We've developed rapid gas- and liquid-phase separation techniques to investigate chemical bonding and periodic trends, successfully measuring the behavior of short-lived isotopes. Our research on dubnium (Db,  $Z=105$ ), for instance, revealed a deviation in volatility from its lighter homologs, as its compounds were more volatile than expected from the periodic table. In a parallel effort, we've launched the "Einsteinium Campaign" using element 99, provided by Oak Ridge National Laboratory, to further explore the nuclear spectroscopy of heavy actinides.

The ISOL (Isotope Separator On-line) system is one of the key apparatus of our research, enabling the production of an ion beam of short-lived heavy element isotopes to investigate atomic properties of these isotopes. By using the system, we've gathered valuable experimental data, including the adsorption and ionization behavior of SHE isotopes.

This presentation will provide an overview of our key findings at JAEA. We will also discuss our future plans, which include the development of next-generation chemical separation systems and the expansion of our ISOL-based studies.



## Chemistry of SHE at GSI: from nihonium, flerovium and moscovium towards livermorium

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The study of superheavy elements has been one of the fundamental pillars of research at GSI. Recent experiments have focused on studying the chemical reactivity of the superheavy 7p-elements nihonium ( $Z = 113$ ), flerovium ( $Z = 114$ ) and moscovium ( $Z = 115$ ) produced in nuclear fusion reactions with heavy-ion beams delivered by the UNILAC accelerator. Ions recoiling from the target are separated in the gas-filled separator TASCA and guided into a recoil transfer chamber that forwards the ions to the chemistry setups COMPACT and miniCOMPACT. These allow studying the adsorption of the elements on gold and  $\text{SiO}_2$  surfaces through gas-solid chromatography. In these experiments, nihonium and moscovium were found to be significantly more reactive than their neighbour flerovium. Quantum chemical theoretical calculations allow explaining this via the influence of strong relativistic effects on the valence electron orbitals of the elements. On the way to chemical studies of the next heavier elements, livermorium and beyond, new challenges need to be overcome as the half-lives of even the most long-lived known isotopes are below 100 ms and production cross sections decrease significantly. The study of these elements thus demands a fast and efficient extraction of ions into chemistry setups. To minimize the transport time of short-lived nuclei into chemistry setups, the buffer gas cell UniCell, which will serve as a link between the pre-separator and the chemistry setup, is currently being constructed. To further prepare future studies of livermorium and tennessine and to obtain guidance from trends in the periodic table, their lighter homologues polonium and astatine need to be studied. We have thus investigated the chemical behaviour of polonium and astatine in the atom-at-a-time regime by applying the same chemical methods as for superheavy elements. These experiments, together with the ongoing technical development of UniCell, lay the foundation for future investigations of the superheavy 7p-elements from livermorium onwards, further advancing the frontier of heavy-element research.

## Some possible ways to produce superheavy nuclei

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The synthesis of superheavy nuclei remains challenging in nuclear physics, aiming to extend the periodic table and exploring the limits of nuclear stability. To synthesize new superheavy nuclei and reach the predicted “island of stability”, fusion reactions have been experimentally and theoretically investigated. The traditional methods of achieving new superheavy nuclei through cold and hot fusion reactions face a significant hurdle due to their low production cross sections. In this presentation, some possible ways, such as the proper projectile target combinations with optimal incident energies for the fusion reactions and for the multinucleon transfer reactions, to produce superheavy nuclei are presented.

## Exotic decays in open quantum systems

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Resonances—quantum states with unbound character and finite lifetimes—are fundamental features of systems that extend beyond the closed-boundary approximation. They manifest across a broad spectrum of physical systems, from hadrons and atoms to exotic nuclear species such as dripline and superheavy nuclei, where they play a crucial role in governing reaction dynamics and decay processes.

Traditionally, the decay of resonant states has been described by the exponential law. However, recent developments in quantum theory have revealed inherent limitations in this description, uncovering rich nonexponential decay behavior, particularly in open quantum systems where coupling to the continuum is essential.

In this presentation, we will begin with a brief overview of the general properties of resonances. Building upon our recent work<sup>1</sup>, we will then explore specific regimes of nonexponential decay. These include the decay of threshold resonances, particle correlations in three-body decays, and interference effects between near-lying resonances. We introduce novel theoretical observables and suggest experimental strategies to probe long-time deviations from exponential decay. These phenomena arise from quantum interference and provide unique insight into the continuum structure of many-body open systems. Our results open new avenues for experimental investigation and deepen our understanding of quantum decay dynamics in resonant environments.

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# Theoretical Studies of the Coordination Structures, Stabilities and Electronic Spectra of Cm<sup>3+</sup> Species at the Mineral-Water Interface

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Accurate interpretation and prediction of actinide coordination chemistry at the mineral-water interface is one of the key scientific issues that need to be urgently addressed in environmental radiochemistry as well as in the safe treatment and disposal of radioactive waste. Various electronic spectroscopic techniques are powerful tools for analyzing the interactions between actinides and minerals in the aqueous environment and revealing the morphology and electronic structure of actinide species. However, due to the complexity of the chemical behaviors of actinides at mineral-water interface, the relevant information derived from experimental spectroscopic data is approximate. And therefore, there is an urgent need for precise simulations at the atomic scale to obtain accurate information. However, due to the strong relativistic and electron correlation effects of actinides, as well as the high complexity of their interactions with mineral surfaces, high-precision theoretical calculations of actinides at mineral-water interface are extremely challenging and rarely reported. In particular, no theoretical studies of the electronic spectra of actinides at the mineral-water interface have been carried out.

In this talk, we will report theoretical investigations of the coordination chemistry of trivalent curium ion at typical mineral-water interfaces by combining ab initio molecular dynamics (AIMD) simulations and static calculations (including static density functional theory calculations and wave function theory calculations)<sup>1-3</sup>. The coordination structure, thermodynamic and kinetic stability, and electronic spectral properties of Cm<sup>3+</sup> sorption species have been accurately predicted, with the calculation results in good agreement with available experimental results. Besides, the effective computational strategies applicable to studying the interaction between actinide ions and mineral surfaces in the aqueous environment have been proposed.

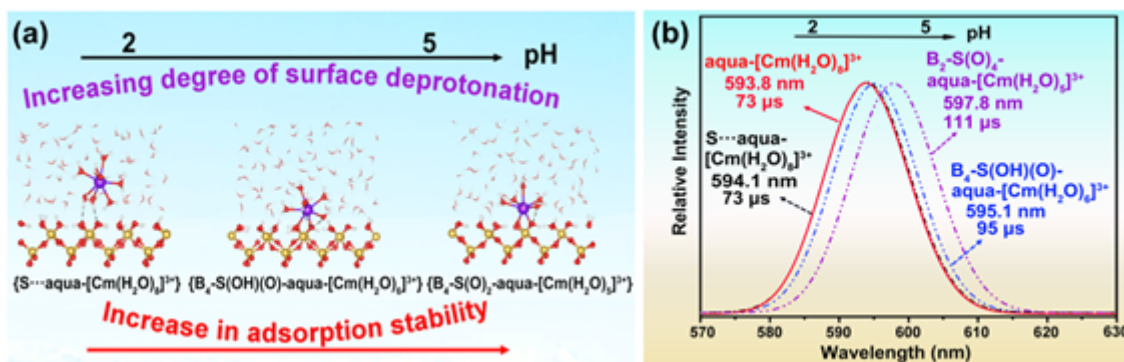


Figure 1. Calculation results for the stable Cm<sup>3+</sup> aqua ion and inner-sphere sorption species at the hydroxylated  $\alpha$ -SiO<sub>2</sub>(001)-water interface: (a) their stability trend with the degree of surface deprotonation and (b) their simulated emission spectra.

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## Theoretical study of adsorptions of superheavy elements and their compounds on various surfaces

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Adsorption energies,  $E_{\text{ads}}$ , of a superheavy element Lv and its lighter homolog Po, as well as of their oxides, hydrides and hydroxides on various modified quartz surfaces are calculated using a periodic density functional theory. Calculations have shown that elemental Po and Lv should be the most volatile over the quartz surface out of all the considered species, with  $E_{\text{ads}}$  of the order of van der Waals bond energies. Hydrides of Po and Lv should be less volatile than the elements. Hydroxides and oxides, particularly dioxides, of these elements should be the least volatile.

Chiera and coauthors<sup>1</sup> reported the experiment focused on adsorption behavior of elemental Hg also on the trigonal Selenium (t-Se) using gas chromatographic methods in order to prepare sensitive chemical separation and characterization of Cn and Fl. To assist this experiment, we calculated adsorption energies of Group-12 (Hg, Cn) and of Group-14 (Pb, Fl) elements using periodic relativistic DFT methods. Our theoretical results show that the adsorption energies of Hg, Cn elements are close to each other. Adsorption energies of Group-12 elements are lower than the adsorption energies of Group-14 elements. Therefore, in the future experimental separation and characterization the elemental Cn should be distinct from the elemental Fl on the t-Se surface.

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## Relativistic periodic calculations of adsorption properties of superheavy elements and their homologs on the surfaces of gold

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Relativistic periodic DFT calculations were performed to predict the adsorption energies,  $E_{\text{ads}}$ , of 7p superheavy elements (SHEs) and their lighter homologues on the gold surface. Adsorption energies were also obtained for their most likely accompanying species, including hydrides, oxides, and oxyhydrides. The unique chemical behavior of the SHEs is governed by the large spin-orbit (SO) splitting of the 7p atomic orbitals (AO), as well as stabilization and destabilization of the  $7p_{1/2}$  AO and  $7p_{3/2}$  AOs, respectively.

According to the results, the most volatile elemental SHEs are Cn, Fl, and Og. Cn and Og have closed 7s and 7p electron shells, respectively, while the high volatility of Fl is attributed to the large SO splitting that results in a quasi-closed  $7p_{1/2}$  electron shell. For elemental SHEs, the calculated  $E_{\text{ads}}$  sequence is  $\text{Cn} < \text{Og} < \text{Fl} < \text{Nh} < \text{Ts} < \text{Mc} < \text{Lv}$ . The majority of the studied compounds exhibit much stronger interactions with the gold surface, identifying them as highly reactive species.

This study provides a comprehensive set of theoretical data to support future one-atom-at-a-time gas-phase chromatography experiments aimed at investigating the reactivity/volatility of SHEs.

**Co-authors:** Nikita Dulaev (Department of Physics, St. Petersburg State University), Miroslav Iliaš (BLTP JINR Dubna, Russia), Vladimir Shabaev (St. Petersburg State University)

## Theoretical issues towards the synthesis of superheavy new elements

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The synthesis of new superheavy elements beyond  $Z = 118$  has extremely low cross sections. Therefore, the choice of beam energies is of vital importance and in this perspective, the reliable theoretical predictions of masses and fission barriers of superheavy region are very needed. Since there are no experimental nuclear masses above  $Z = 110$ , we include the alpha decay energies up to  $Z = 118$  to optimize the energy density functional, so that we obtain very high quality microscopic nuclear masses in the heaviest region. This will be useful for determining the reaction  $Q$  values. In addition, we performed self-consistent calculations of energy dependent fission barriers with quadrupole, triaxial and octupole deformations. Then we calculate the survival probabilities and the residual cross sections to predict the optimal beam energies for synthesizing  $Z = 119$  element.

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## Extended Monte-Carlo model for SHE adsorption simulation

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We developed a new model for simulation of SHE adsorption on a gold surface, combining quantum chemical and molecular dynamics approaches with gas-dynamic modeling and experimental parameters. This model considers atomic motion in the gas phase as well as the interaction between SHE atoms and surfaces in a more general and rigorous way than the existing mobile adsorption model. The developed method was applied to interpret the experimental results of Cn and Fl adsorption on gold obtained at FLNR.

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## Diffusion Control as part of Monte-Carlo simulation of gas chromatography

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Recently, results from ultrafast gas phase chemistry experiments have been presented for the elements Nh and Mc using chromatography detectors, which are directly attached to the recoil transfer chambers, mounted at the focal plane of physical pre separators<sup>1,2</sup>. In preparation of these, experiments with lighter homologues of transactinides have been performed at high statistical confidence but at otherwise same experimental conditions<sup>3,4</sup>. The recently observed deposition patterns for SHE and their lighter homologues with in part unknown chemical speciation are not well reproduced by the corresponding Monte-Carlo simulations involving empirical models for gas transport dynamics and diffusion<sup>5</sup> with partly great implications on the evaluated adsorption data for the investigated chemical species on the detector surface materials SiO<sub>2</sub> and Si<sub>3</sub>N<sub>4</sub>.

Here, we would like to revisit the deposition patterns of gas phase species under isothermal conditions and in temperature gradients in square channel column geometries<sup>5,6</sup>. We would like to summarize the difficulties and try to suggest approaches, that could be used to tackle the discrepancies between the experiments at stable conditions and the model predictions at the exactly same conditions. Thus the aim of this talk is to initiate a community-wide discussion on how to address such effects and try to learn how to perform concise data analyses for the experiments at hand.

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## Upgrade of the Cryodetector setup for study the gas-phase chemistry of Cn and Fl behind the GRAND separator

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The study of Fl chemistry is important because of its controversial behaviour in gas chromatography experiments, as well as discrepancies in theoretical predictions of the adsorption enthalpy of Fl on gold and periodic trends<sup>1</sup>. In order to resolve this issue, one needs to conduct new experiments with higher statistics. A new gas-filled recoil separator GRAND was built at the SHE Factory to provide physical separation of the desired ions with the highest efficiency possible for further experiments in physics and chemistry. The setup created for studying the chemistry of Nh was modernized to meet the requirements for experiments with Fl<sup>2,3</sup>. The improved setup called Cryodetector consists of the RTC filled with an inert gas mixture to stop and thermalise all the reaction products coming from the GRAND separator through a thin film separating gas volume of the Cryodetector from the low pressure of the separator (0.7 Torr); gas transportation and purification system to transport volatile species formed in the RTC to the detector assembly with applied temperature gradient to adsorb the studied species at a temperature. Improvements included developing a new RTC based on recoil stopping range measurements, manufacturing new gold coated detectors, extending the linear temperature gradient from room temperature to  $-170\text{ }^{\circ}\text{C}$ , implementing a closed gas loop, and replacing all components of the measurement system with new high-quality electronics for better resolution. The setup coupled with GRAND was tested in on-line experiments using short-lived radioisotopes  $^{178,179}\text{Hg}$  produced in  $^{144}\text{Sm}(^{40}\text{Ar},\text{xn})$  reactions. Experimental results of collecting recoil atoms of Hg and No in different He and Ar gas mixtures are presented. A median transport time 0.2 s was achieved, which is shorter than  $^{287}\text{Fl}$  half-life and leads to a significant increase in transport efficiency. The test results demonstrated the setup readiness for gas adsorption thermochromatography experiments with  $^{287}\text{Fl}$  behind the GRAND separator.

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## High-resolution internal conversion electron spectroscopy for superheavy nuclei

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The stability of superheavy nuclei (SHN) essentially depends on nuclear shell structure. One of the most sensitive probes to clarify the shell structure is energy spacing and order of proton and neutron single-particle orbitals which can be deduced from level structure of ground and excited states in nuclei. To establish level structure of SHN, alpha-gamma coincidence spectroscopy is very powerful and sensitive. However, since the alpha decays favor the population of low-energy excited states in daughter nuclei, following gamma transitions should have low energy and thus large internal conversion coefficients. This makes gamma-ray spectroscopy of SHN extremely difficult because gamma-ray emission probabilities become very low. Internal conversion electron (ICE) spectroscopy is an alternative method to study level structure of SHN, although its application to SHN<sup>1,2</sup> is scarce because of difficulties in measuring low-energy electrons with high energy resolution and low signal-to-noise ratio. The aim of the present study is to realize ICE spectroscopy of SHN, where we aim at measuring low-energy electrons of SHN down to  $< 10$  keV with extremely high energy resolution of  $< 0.5$  keV FWHM. Previously we successfully measured ICE following the alpha decay of No-257 using Si PIN photodiode detectors<sup>1</sup>, although the energy resolution is only  $\sim 2$  keV FWHM. In the present work, we tested a silicon drift detector which is typically used to measure low-energy X rays in synchrotron radiation experiments and X-ray fluorescence analysis. We applied this detector to measure low-energy ICE, and investigated their energy resolutions and applicability of this detector to the spectroscopy of SHN.

**Co-authors:** MIYASHITA, Naoto (Kyushu University)

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## Design and fabrication of 4H-SiC detectors for Nh study

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The study of chemical properties of superheavy elements (SHEs) is one of the advanced topics in fundamental research field, aiming at exploring the insights of the Periodic Table of chemical elements and developing new technologies. As one of the heaviest elements which can be chemically studied, the experimental study of nihonium (Nh,  $Z = 113$ ) chemistry has great research value in the field of nuclear chemistry. The passive implanted planar silicon (PIPS) detectors are commonly used to detect high-energy alpha particles released by the cascade decay of Nh elements, to obtain chemical information such as adsorption enthalpy combined with method of thermal chromatography. However, the temperature gradient field of the current testing system is limited due to the inability of silicon-based PIPS detectors to operate stably at temperatures above 50 °C. Therefore, the development of new advanced detection technologies suitable for higher temperatures is urgent for acquiring of more accurate measurement of the chemical properties of the Nh element. The wide bandgap semiconductor 4H-SiC has characteristics such as high displacement threshold energy and high thermal conductivity, making it a good choice to replace traditional Si based detectors. This study aims to develop a high-performance 4H-SiC detector for meeting the research needs of the Nh element. The main contents will be discussed in this report as follows: 1) Schottky Barrier Diode type 4H-SiC (SiC-SBD) detectors were designed and fabricated for the detection of high-energy alpha particles with a thin layer of SiN<sub>x</sub> film as surface coverage, and integrated as a long row detector array. The energy resolution of the detectors was found generally better than 1.5% @ 5486 keV at 80 °C with well consistency via the experimental tests, which indicates that the fabricated 4H-SiC detector can meet the requirements of thermal chromatography testing up to a temperature of 80 °C. 2) Metal semiconductor metal type 4H-SiC (SiC-MSM) detectors were also prepared to further enhance their high-temperature performance. The test results show that the energy resolution of SiC-MSM detector at room temperature is about 1.2%, gradually deteriorated as the temperature increases, but the detector can still operate stably with an energy resolution of about 3.0% under the temperature environment of 300 °C. However, the energy resolution of SiC-SBD detectors had decreased to about 5.1% at 200 °C, and facing challenges of higher noise levels under higher temperature above 200 °C environmental conditions. Current research indicates that SiC-MSM detectors

are more suitable for studying SHEs with higher temperature requirements. This study provides important technical references for the development of high-performance detectors for the study of SHEs.

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**Key words:** 4H-SiC; superheavy elements; detector; high temperature; energy resolution

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## Spectroscopy of neutron-rich nuclei produced by multinucleon transfer reactions

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Multinucleon transfer (MNT) reactions have recently attracted renewed attention due to their potential to synthesize neutron-rich nuclei around  $N = 126$  and actinides, which are relevant for elucidating r-process<sup>1</sup>. In MNT reactions, a wide variety of nuclei are produced around both the projectile and the target nuclei, which a wide range of angular and energy distributions, so in order to perform spectroscopy experiments on specific reaction products, it is essential to develop experimental techniques to collect, separate, and identify them. In particular, exotic nuclei far from the projectile or target are produced so infrequently that they can get buried among more abundant reaction products. Rapid separation is particularly important for short-lived nuclei with lifetimes of less than a few minutes.

At the RIKEN Nishina Center, we are developing the KEK Isotope Separation System (KISS) to extract MNT reaction products and perform their spectroscopic studies<sup>2</sup>. The system combines an argon-gas-cell-based laser ion source with an online isotope separator. MNT reaction products are thermalized and neutralized in argon gas, element-selectively ionized, and mass-separated by a dipole magnetic field. We perform decay and laser spectroscopy, and mass spectrometry of neutron-rich nuclei of refractory elements around the  $N = 126$  region. Recently, our work has been extended to atomic mass spectrometry of neutron-rich actinides using a  $^{238}\text{U}$  beam<sup>3</sup>.

In this presentation, we will report on the KISS experimental methods and results, as well as future development plans for further neutron-rich regions.

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## MRTOF mass spectrometer at SHANS for fusion-evaporation residues

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To precisely measure atomic masses and select neutron-deficient isotopes produced by fusion evaporation reactions, a multi-reflection time-of-flight mass spectrometer (MRTOF-MS) at Spectrometer for Heavy Atom and Nuclear Structure (SHANS) is being developed at the Institute of Modern Physics, Chinese Academy of Sciences. SHANS is a gas-filled recoil separator. In recent years, several new isotopes in the actinide region have been synthesized and their decay properties studied experimentally at SHANS<sup>1</sup>.

The MRTOF-MS consists of three key parts: The cryogenic gas catcher (CGC), the radio-frequency (RF) ion trap system, and the MRTOF mass analyzer. Firstly, the recoils separated by the SHANS are collected by the CGC and transported by the electrostatic field of the DC cage together with a RF carpet. Secondly, the ions extracted out of the gas catcher are accumulated, cooled, and pulsed by the RF ion trap system<sup>2</sup>. At last, the atomic masses are measured by the MRTOF mass analyzer<sup>3</sup>.

All three parts have been constructed, tested separately and commissioned offline and online. In this talk, the design, construction, offline joint commissioning, and online experimental results will be presented in detail.

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## Deformation, deformation energy, and excitation energy in heavy and superheavy nuclei

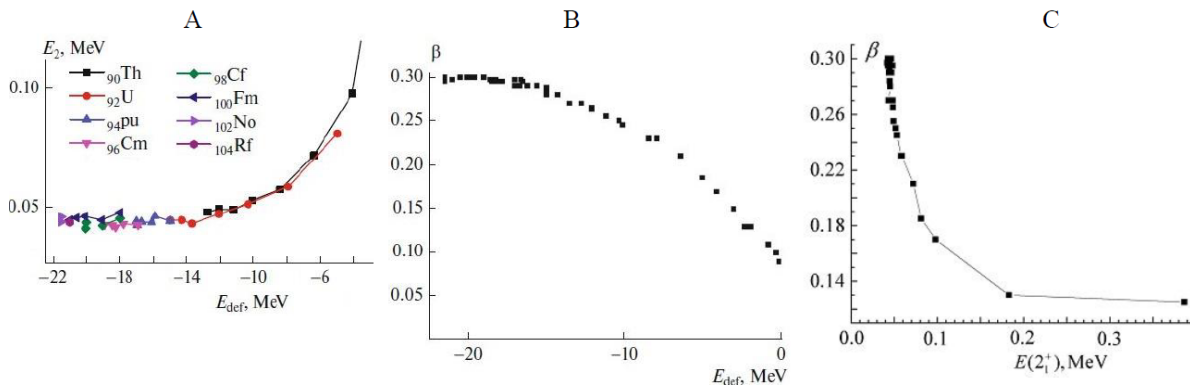
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Judgments about the magnitude of deformation are usually obtained from the value of  $B(E2; 2_1^+ \rightarrow 0_1^+)$ . It is obvious that the deformation parameter, being a model geometric parameter, is associated both with the energy of the lowest excitation and with the nature of the spectrum itself. With increasing deformation, the energies of the main band approach the dependence of the  $I(I+1)$  and never reaching it. For many heavy and superheavy nuclei the value of  $B(E2; 2_1^+ \rightarrow 0_1^+)$  is unknown. However, the estimation of the deformation parameter would be very useful, since as it decreases during the transition from nucleus to nucleus one can judge about the approach to the island of stability<sup>1</sup> for superheavy nuclei. For this purpose, it is necessary to relate the calculated deformation energies, the deformation parameter at which this energy is minimal, and the first excitation energy for nuclei where this energy is known. In this case, it is necessary to use a single model within which deformation characteristics are calculated for the widest range of nuclei. For doing this, the work<sup>2</sup> is used, where the calculation of the deformation energy is carried out in the Hartree–Fock–Bogoliubov scheme with Gogny realistic forces. Using the results of these calculations and the known first excitation energies  $E(2_1^+)$  for some heavy even-even nuclei, the dependence of the  $E(2_1^+)$  on the deformation energy was obtained in [3]. The corresponding systematics constructed from experimental energies (Fig. A and Fig. B) allows us to estimate unknown energies and the deformation parameter  $\beta$  from the deformation energies<sup>4</sup>. However, it is also possible to do the opposite, using only measured energies of the  $E(2_1^+)$  to estimate the deformation parameters<sup>1</sup>. For such estimates, we obtained the corresponding systematics of the dependence of the on the deformation parameter (Fig. C).



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## Liquid-phase separation systems for SHE homologs at the CTU

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The chemical behavior of superheavy elements (SHEs) is of fundamental scientific interest. By means of liquid-liquid extraction, Mo and W (both lighter homologs of Sg,  $Z = 106$ , in group 6) were investigated regarding their behavior at ultra-trace concentrations with non-complexing (e.g., nitric or perchloric acid, where these elements undergo only hydrolysis), and with complexing acids (e.g., hydrochloric and hydrofluoric acid, with which additional complexation occurs). The extractants Cyanex 272 and Aliquat 336 were employed for these studies; Cyanex 272 being an extractant capable of extracting various species has been used universally, while Aliquat 336 has been used solely for extraction of anionic species. In addition, the extraction of anionic chloride species of heavy group 12 (for Cn,  $Z = 112$ ) and 13 (for Nh,  $Z = 113$ ) elements is subject to dedicated studies. In group 13, the use of suitable conditions allows us to separate different oxidation states of Tl formed after electrochemical or chemical pretreatment. Meanwhile, for group 12, extraction properties of various precursors of self-assembled monolayers are studied for subsequent sorption studies.

Lastly, electrochemistry can be employed to study the redox behavior of group 11 elements under non-carrier-added conditions. At these ultra-trace concentrations, the electrochemical behavior is strongly influenced by the electrode surface. In a first attempt, the behavior of the lighter homologs of Rg ( $Z = 111$ ), Ag and Au, are to be experimentally studied for this purpose in parallel to dedicated model developments. Ultimately, these efforts strive for the extraction of meaningful thermochemical data.

Here, various liquid-phase separation systems, that are currently under investigation at the CTU and its collaborating partners, are presented with an emphasis on homologs of Sg, Rg, Cn, and Nh. Selected results, experimental systems and their underlying chemistry will be presented, as well as suggestions on how to exploit some of the findings for SHE research.

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## Extraction behavior of fluoride complex of dubnium with tributyl phosphate

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The extraction behavior of dubnium, the heaviest group-5 element in the periodic table, was investigated using on-line column chromatography with tributyl phosphate (TBP) as an extractant from 1.0 M hydrofluoric acid (HF) solution. The extraction behavior of Db was compared with those of its lighter homologs niobium (Nb) and tantalum (Ta). Ta was efficiently extracted into the TBP-laden resin under these conditions, while both Nb and Db were extracted to a much lesser extent. This similarity between Db and Nb suggests that Db may form oxofluoro complexes in aqueous HF under the studied conditions, in contrast to the homoleptic fluoro complexes likely formed by Ta. Although the exact chemical species of Db remain unclear, the data indicate that Db may behave more like Nb than Ta under these conditions.

To support this interpretation, relativistic DFT calculations were performed using the TPSSH functional, including spin-orbit coupling and solvent effects. The results indicate that the Gibbs free energy changes associated with hydrolysis reactions are less favorable for Db than for Nb or Ta, suggesting that Db is thermodynamically less prone to hydrolysis under the studied conditions. In contrast, the formation of higher coordinate fluoro complexes is relatively favorable for Db. This reveals a clear discrepancy with interpretations based on experimental observations. Additional calculations are ongoing, and their implications for the speciation of Db may be discussed in the presentation.

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## Nobelium Extraction from Nitric Acid with TODGA-resin

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Nobelium (No,  $Z = 102$ ) uniquely exhibits +2 oxidation state in aqueous solutions within the actinide series. The chemical behavior of No resembles that of group 2 elements, but it may have a softer acidic nature. For a systematic chemical study of No, we propose extraction with diglycolamide (DGA) ligands, which allow for various structural modifications to tune their coordination and extraction properties. In this work, we investigated the behavior of group 2 elements and Pb(II) in extraction from nitric acid using TODGA-resin, performed relativistic DFT calculations of the extracted M(II)-DGA complexes, and validated the extraction system for an online experiment with No. The results of the recent experiment on No-255 at RIKEN will also be reported in the presentation, paving the way for further systematic research on No using DGA ligands.

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# Theoretical investigation of the extraction and separation mechanism of Am(III)/Eu(III) by asymmetric extractants

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The effective separation of trivalent actinides (i.e., An(III)) from trivalent lanthanides (i.e., Ln(III)) has long been a critical technical challenge in the closed nuclear fuel cycle due to their highly similar chemical properties. Accordingly, various extractants containing N, O, or S donor atoms have been synthesized and used to selectively separate An(III) from Ln(III). In particular, the N, O-donor extractants that comply with the CHON principle have been extensively studied. However, most reported N, O-donor extractants feature symmetric structures based on pyridine or phenanthroline backbones, whereas studies on asymmetric analogs remain limited. In this work, three asymmetric extractants, which possess an N-heterocyclic backbone functionalized with amide and triazine side chains (Figure 1), were designed and investigated by combining theoretical calculations and experimental studies. We systematically evaluated the extraction and separation performance of the three asymmetric extractants for Am(III)/Eu(III) through chemical bonding analyses and thermodynamic calculations at the DFT level of theory. Computational results revealed that the Et-Tol-CyMe<sub>4</sub>-ATPhen (L3) ligand exhibited the strongest extraction and separation capability, which was further validated by subsequent experimental results. This work not only deepens our understanding of the coordination chemistry underlying Am(III)/Eu(III) separation (as a representative pair of An(III)/Ln(III)), but also highlights the critical role of integrating theoretical calculations with experimental studies in the development of efficient metal separation extractants.

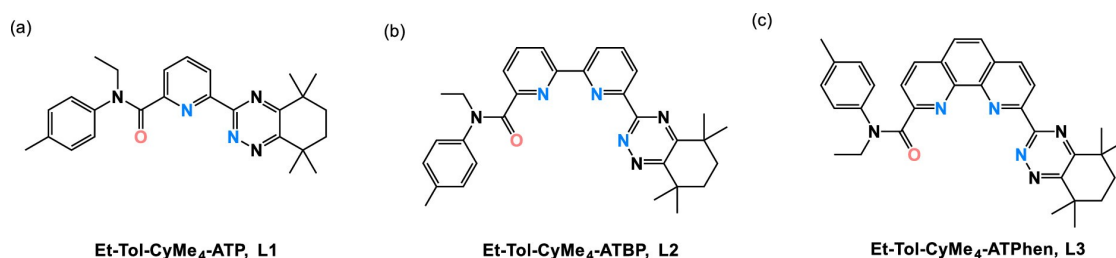


Figure 1. Molecular structures of the three asymmetric extractants.

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