

PSI Center for Nuclear Engineering
and Sciences

From Polonium to Nihonium

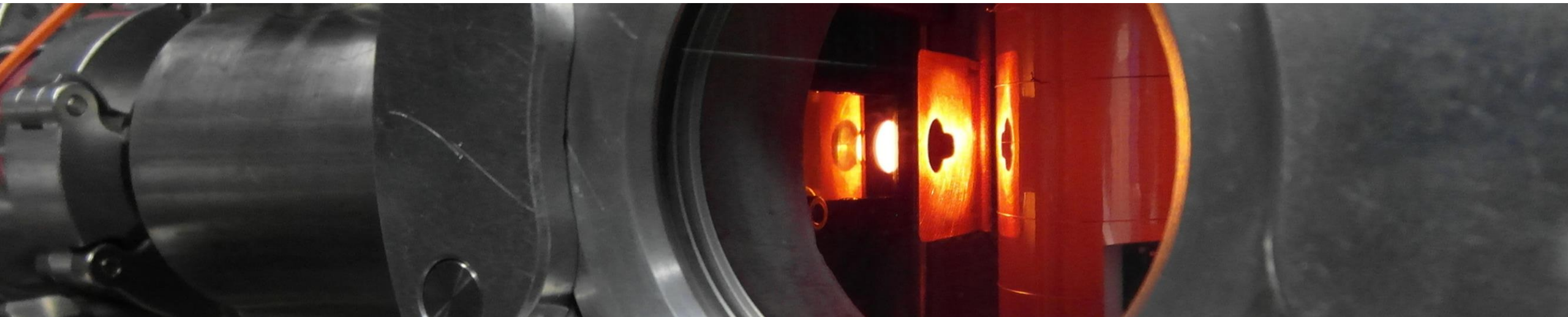
Radiochemical Research at
the Paul Scherrer Institute

Patrick Steinegger (PSI / ETHZ)

European Summer School, Strasbourg, France, 01 – 05 July 2024

Agenda

- 1 Why do we need Radiochemistry?
- 2 The Laboratory of Radiochemistry
- 3 Radionuclide Production at PSI
- 4 Chemistry Experiments with Superheavy Elements
- 5 The Chemistry of Gen IV nuclear reactors



Why do we need Radiochemistry?

1 H hydrogen 1.0080 ± 0.0002																	2 He helium 4.0026 ± 0.0001
3 Li lithium 6.94 ± 0.06	4 Be beryllium 9.0122 ± 0.0001																
11 Na sodium 22.990 ± 0.001	12 Mg magnesium 24.305 ± 0.002																
19 K potassium 39.098 ± 0.001	20 Ca calcium 40.078 ± 0.004	21 Sc scandium 44.956 ± 0.001	22 Ti titanium 47.867 ± 0.001	23 V vanadium 50.942 ± 0.001	24 Cr chromium 51.996 ± 0.001	25 Mn manganese 54.938 ± 0.001	26 Fe iron 55.845 ± 0.002	27 Co cobalt 58.933 ± 0.001	28 Ni nickel 58.693 ± 0.001	29 Cu copper 63.546 ± 0.003	30 Zn zinc 65.38 ± 0.02	31 Ga gallium 69.723 ± 0.001	32 Ge germanium 72.630 ± 0.008	33 As arsenic 74.922 ± 0.001	34 Se selenium 78.971 ± 0.008	35 Br bromine 79.904 ± 0.001	36 Kr krypton 83.798 ± 0.002
37 Rb rubidium 85.468 ± 0.001	38 Sr strontium 87.62 ± 0.01	39 Y yttrium 88.906 ± 0.001	40 Zr zirconium 91.224 ± 0.002	41 Nb niobium 92.906 ± 0.001	42 Mo molybdenum 95.95 ± 0.01	43 Tc technetium [97]	44 Ru ruthenium 101.07 ± 0.02	45 Rh rhodium 102.91 ± 0.01	46 Pd palladium 106.42 ± 0.01	47 Ag silver 107.87 ± 0.01	48 Cd cadmium 112.41 ± 0.01	49 In indium 114.82 ± 0.01	50 Sn tin 118.71 ± 0.01	51 Sb antimony 121.76 ± 0.01	52 Te tellurium 127.60 ± 0.03	53 I iodine 126.90 ± 0.01	54 Xe xenon 131.29 ± 0.01
55 Cs caesium 132.91 ± 0.01	56 Ba barium 137.33 ± 0.01	57-71 lanthanoids	72 Hf hafnium 178.49 ± 0.01	73 Ta tantalum 180.95 ± 0.01	74 W tungsten 183.84 ± 0.01	75 Re rhenium 186.21 ± 0.01	76 Os osmium 190.23 ± 0.03	77 Ir iridium 192.22 ± 0.01	78 Pt platinum 195.08 ± 0.02	79 Au gold 196.97 ± 0.01	80 Hg mercury 200.59 ± 0.01	81 Tl thallium 204.38 ± 0.01	82 Pb lead 207.2 ± 1.1	83 Bi bismuth 208.98 ± 0.01	84 Po polonium [209]	85 At astatine [210]	86 Rn radon [222]
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Key:

atomic number
Symbol
name
abridged standard
atomic weight



INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

57 La lanthanum 138.91 ± 0.01	58 Ce cerium 140.12 ± 0.01	59 Pr praseodymium 140.91 ± 0.01	60 Nd neodymium 144.24 ± 0.01	61 Pm promethium [145]	62 Sm samarium 150.36 ± 0.02	63 Eu europium 151.96 ± 0.01	64 Gd gadolinium 157.25 ± 0.03	65 Tb terbium 158.93 ± 0.01	66 Dy dysprosium 162.50 ± 0.01	67 Ho holmium 164.93 ± 0.01	68 Er erbium 167.26 ± 0.01	69 Tm thulium 168.93 ± 0.01	70 Yb ytterbium 173.05 ± 0.02	71 Lu lutetium 174.97 ± 0.01
89 Ac actinium [227]	90 Th thorium 232.04 ± 0.01	91 Pa protactinium 231.04 ± 0.01	92 U uranium 238.03 ± 0.01	93 Np neptunium [237]	94 Pu plutonium [244]	95 Am americium [243]	96 Cm curium [247]	97 Bk berkelium [247]	98 Cf californium [251]	99 Es einsteinium [252]	100 Fm fermium [257]	101 Md mendelevium [258]	102 No nobelium [259]	103 Lr lawrencium [262]

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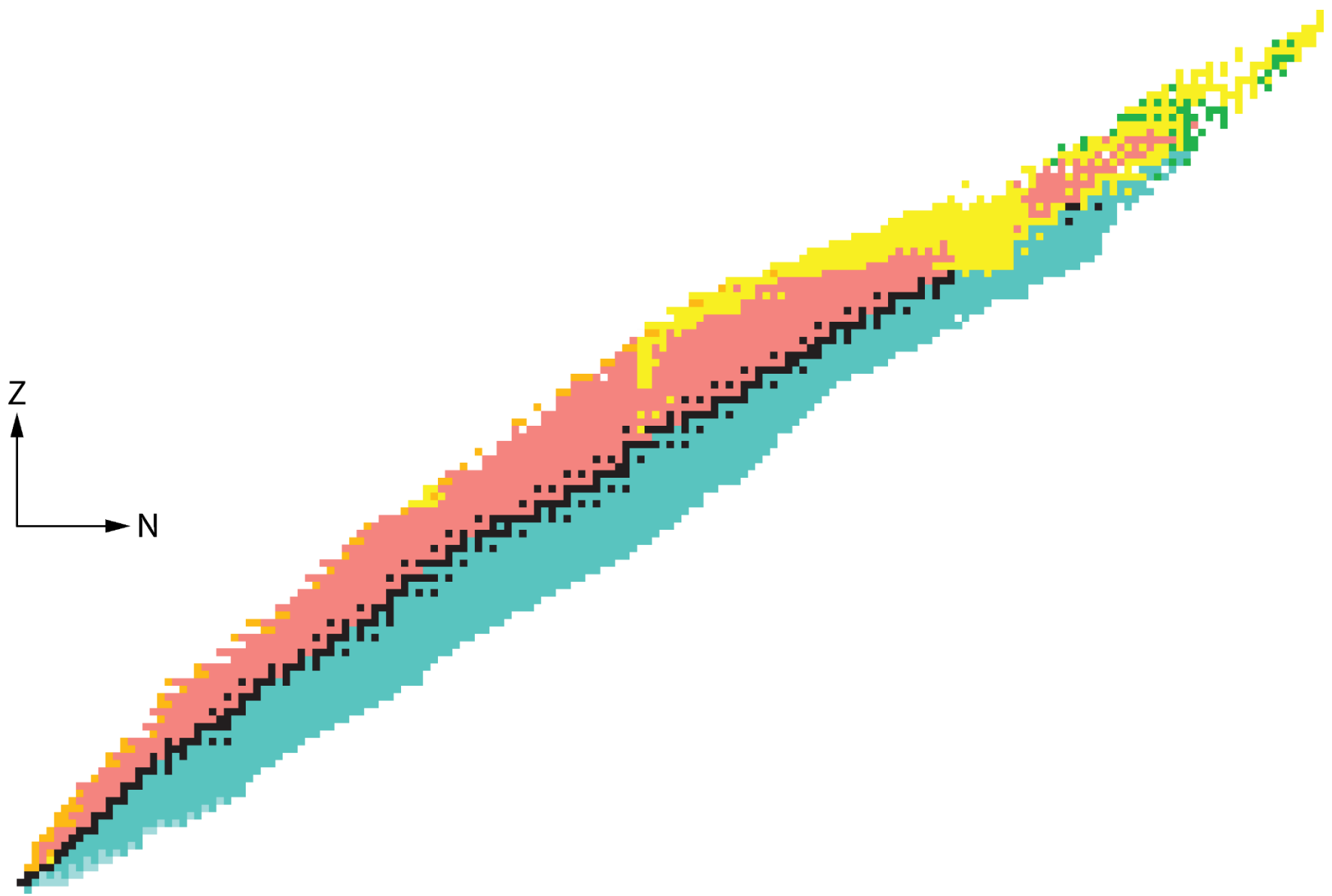
atomic number
Symbol
name
abridged standard
atomic weight



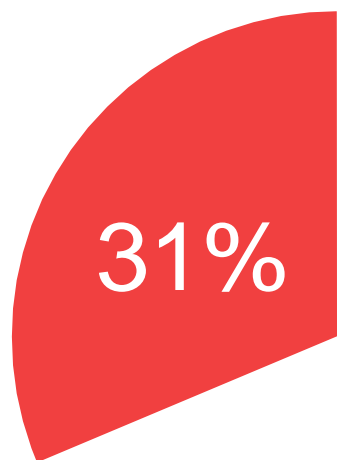
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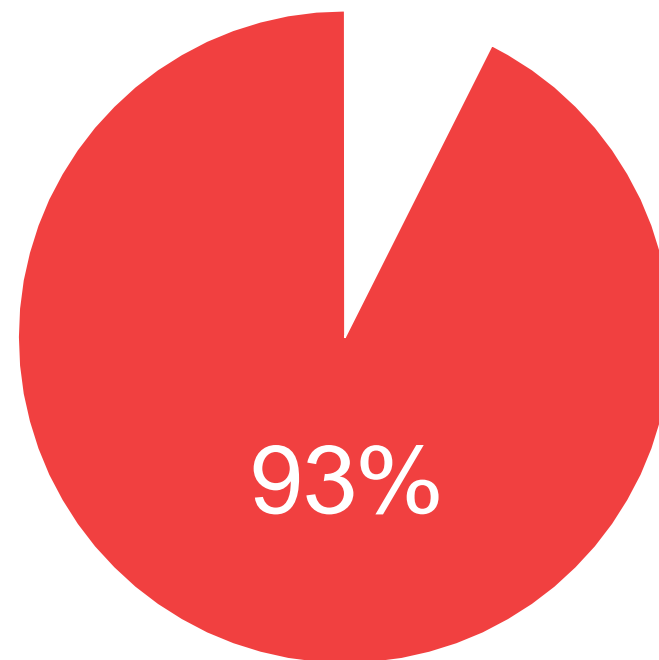
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Radioelements
Stable elements



Radioisotopes
Stable isotopes



The Laboratory of Radiochemistry




ETH zürich

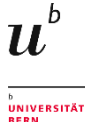
u^b

UNIVERSITÄT
BERN

The Laboratory of Radiochemistry



Prof. Dr. Robert Eichler




Postdoctoral researchers

PhD students

Sandha Keller (Admin, 80%)
Deputy lab head (tbd)

ETH zürich

HEAVY ELEMENTS
Prof. Dr. Patrick Steinegger




Dr. Rugard Dressler
Alexander Vögele
Dominik Herrmann

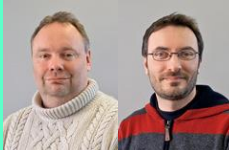


Jennifer Wilson (SNF)
Georg Tiebel (SNF)
Paul Dutheil (ENSI, LOG)
Michael Hofstetter (BABS)
Aleksandr Kharchenko (Uni Basel)

ISOTOPE & TARGET CHEMISTRY
Dr. Zeynep Talip



Dr. Jörg Neuhausen
Dr. Emilio Maugeri
Dr. Djordje Cvjetinovic
Dr. Haohan Zhang




Ivan Zivadinovic (EU, PATRICIA)
Noemi Cerboni (PSI)
Vladislav Zobnin (EU, PASCAL)
Xuandong Kou (Uni Bern)
Elizaveta Artiushova (SwissNuclear)

RADIONUCLIDE DEVELOPMENT
Dr. Nick van der Meulen



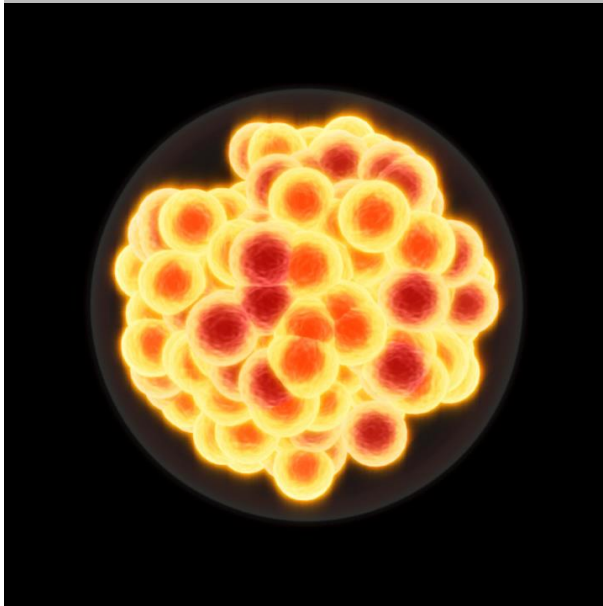
Dr. Who (CRS, BIO)
Dr. Pascal Grundler (CRS, BIO)
Colin Hillhouse (ITM)
Dr. Anzhelika Moiseeva
Dr. Maryam Mostamand



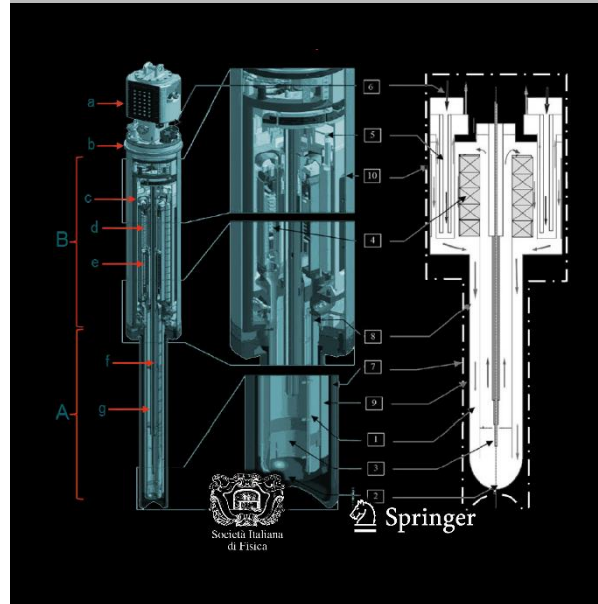
Edoardo Renaldin (Uni Bern)

+ 2 to 3 Master- / Bachelor- / semester students

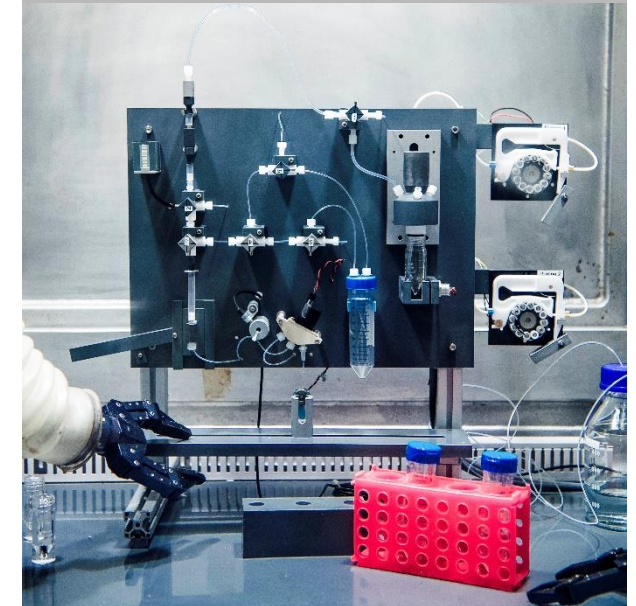
Heavy Elements



Isotope and Target Chemistry



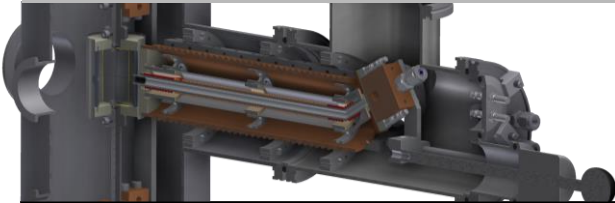
Radionuclide Development



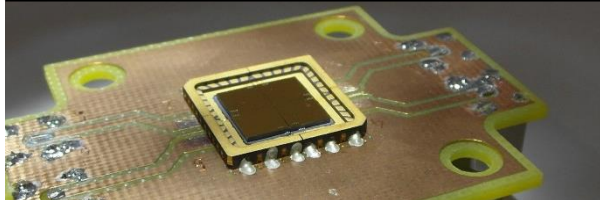
Heavy
Elements

Isotope and Target
Chemistry

Radionuclide
Development



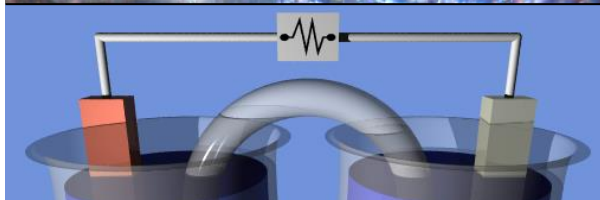
Gas adsorption chromatography with transactinide elements



Detector development for extreme conditions



Targets for heavy ion beam irradiations



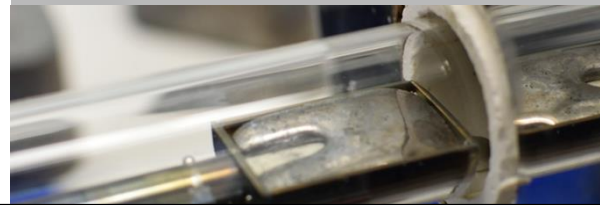
Electrochemistry with transactinide elements

Heavy
Elements

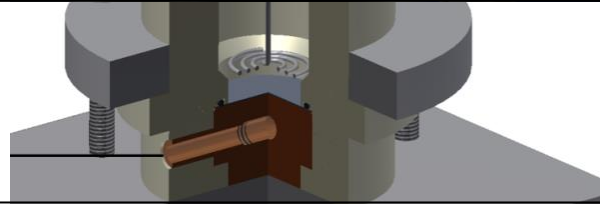
Isotope and Target
Chemistry

Radionuclide
Development

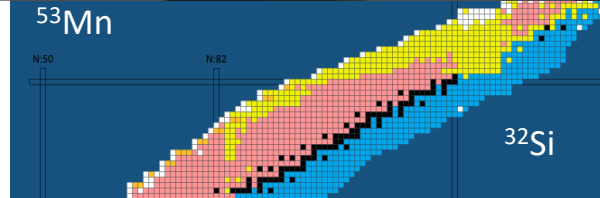
Liquid metal chemistry



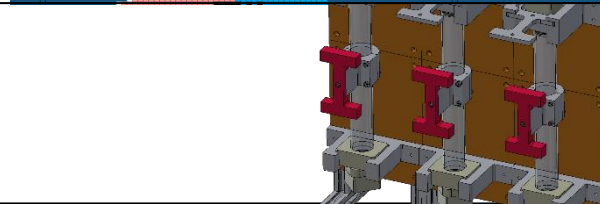
Isotope extraction and target manufacturing



Improvement of nuclear physics data



Waste treatment and isotope reclamation



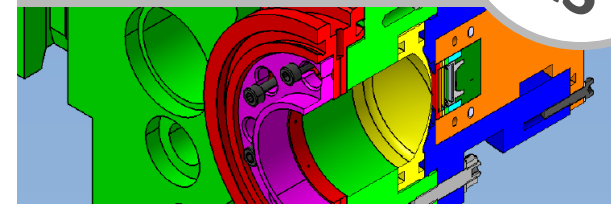
Heavy
Elements

Isotope and Target
Chemistry

Radionuclide
Development

LRC
+
CRS

Target Development



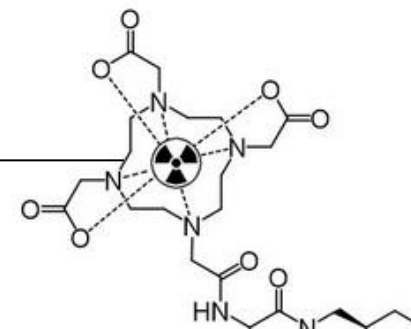
Production of new radionuclides



Chemical separation and processing



Theragnostics

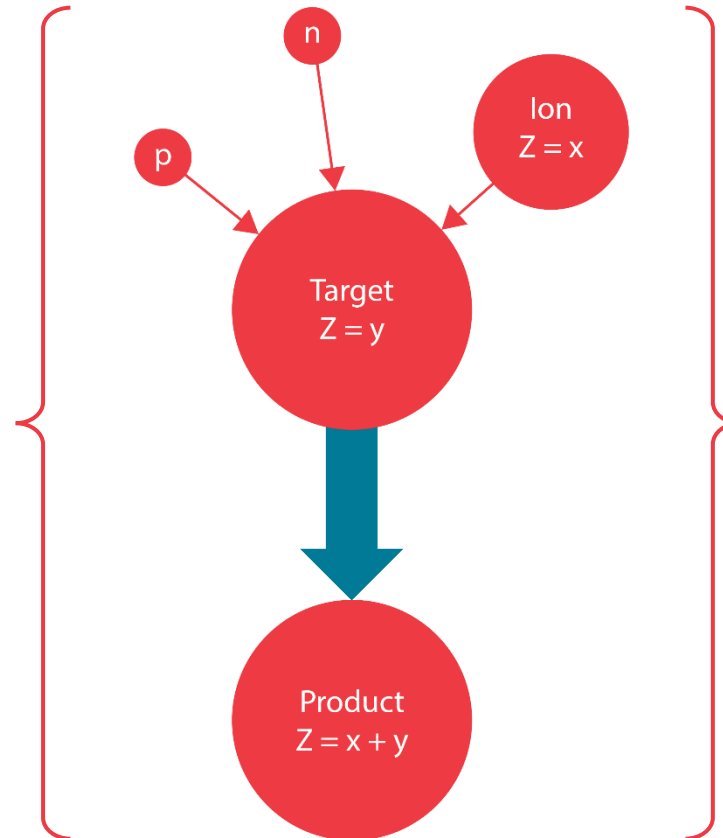


Radionuclide Production at PSI (and elsewhere)

Radionuclide Production at PSI (and elsewhere)



- > **Long-lived** radionuclides (h/d)
- > **Offline** separation procedures



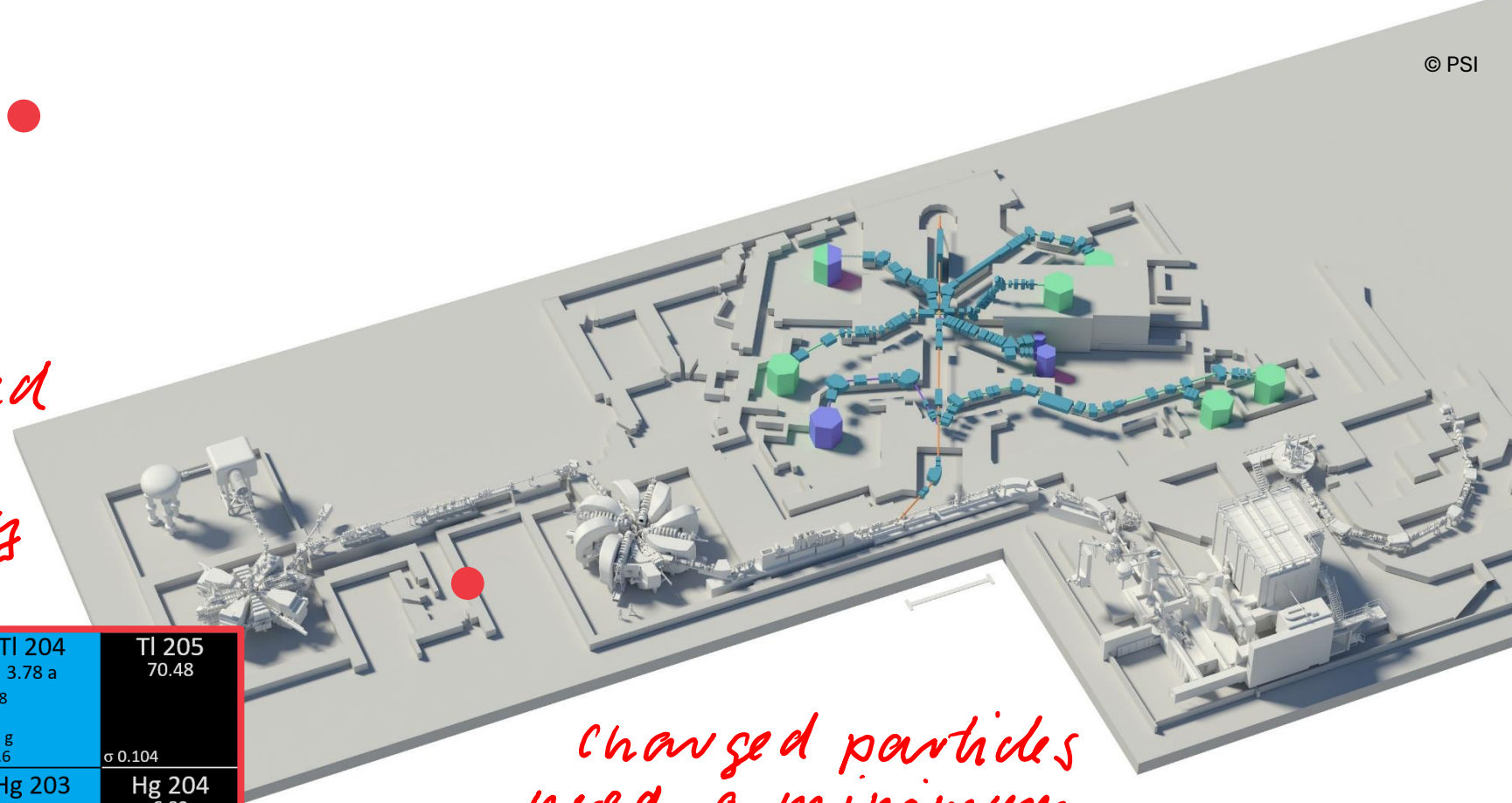
- > **Short-lived** radionuclides (s)
- > **Online** separation procedures



Why is our group at PSI?

- Proton irradiation (72 MeV) ●

number of evaporated neutrons depends on the initial energy of the proton beam



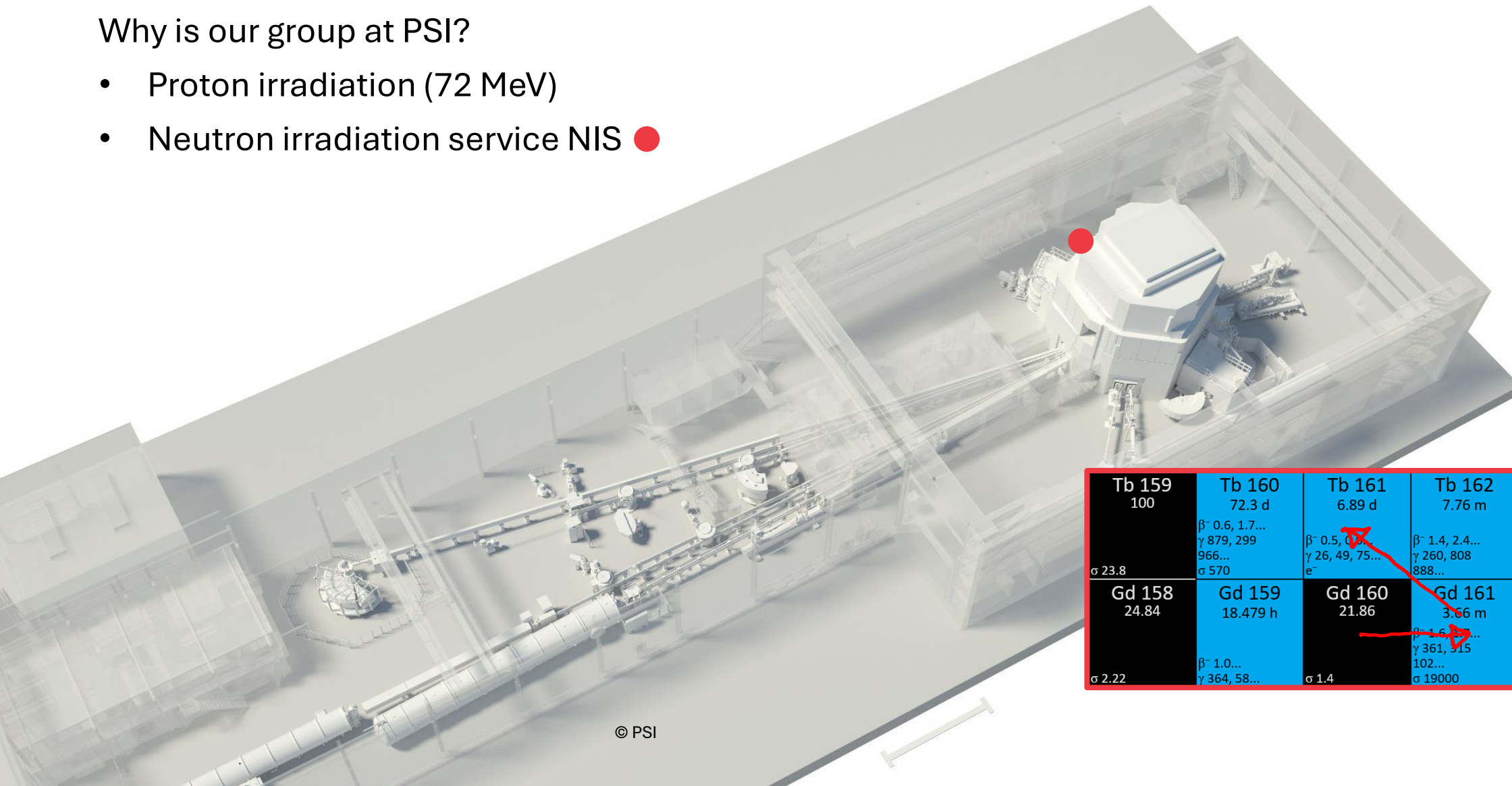
Tl 200 26.1 h ϵ β^+ ... γ 368, 1206, 579 828...	Tl 201 3.0422 d ϵ γ 167, 135...	Tl 202 12.23 d ϵ γ 440, (520...)	Tl 203 29.52 σ 11.4 $\sigma_{n,\alpha} < 0.0003$	Tl 204 3.78 a β^- 0.8 ϵ $n\alpha\gamma, g$ σ 21.6	Tl 205 70.48 σ 0.104
Hg 199 42.67 m 16.94 IT 374... e^- γ 158... σ 2150	Hg 200 23.14 σ 15.0	Hg 201 13.17 σ 4.9	Hg 202 29.74 σ 4.91	Hg 203 46.59 d β^- 0.2 γ 279	Hg 204 6.82 σ 0.43

charged particles need a minimum energy to overcome the Coulomb barrier.

Radionuclide Production at PSI

Why is our group at PSI?

- Proton irradiation (72 MeV)
- Neutron irradiation service NIS ●



Tb 159 100 σ 23.8	Tb 160 72.3 d β^- 0.6, 1.7... γ 879, 299 966... σ 570	Tb 161 6.89 d β^- 0.5, 0... γ 26, 49, 75... e^-	Tb 162 7.76 m β^- 1.4, 2.4... γ 260, 808 888...	Tb 163 19.5 m β^- 0.8, 1.3... γ 351, 390 494...
Gd 158 24.84 σ 2.22	Gd 159 18.479 h β^- 1.0... γ 364, 58...	Gd 160 21.86 σ 1.4	Gd 161 3.66 m β^- 1.6, 3... γ 361, 315 102... σ 19000	Gd 162 8.2 m β^- 1.0... γ 442, 403...

Radionuclide Production at PSI

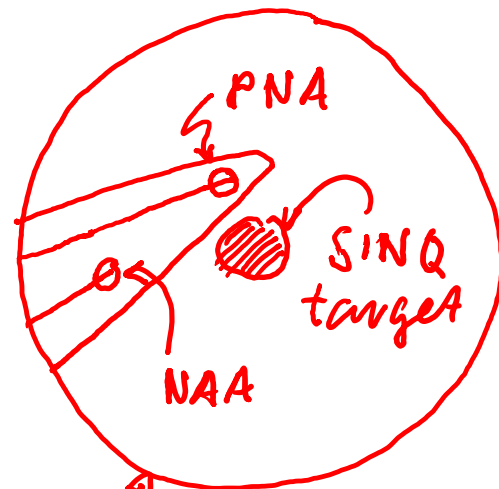
Two irradiation positions for longer irradiation times (PNA; up to 1000 h) and one for shorter irradiations (NAA; up to 2 h).



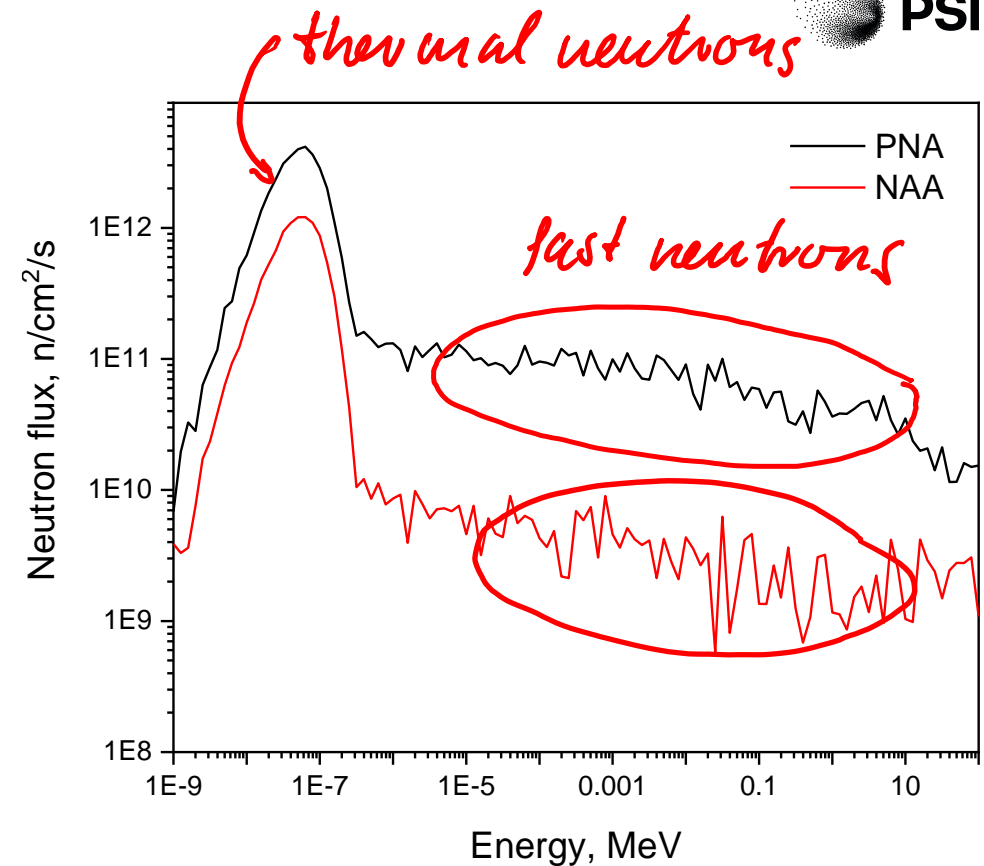
NAA



PNA



Neutron spallation source seen from top.

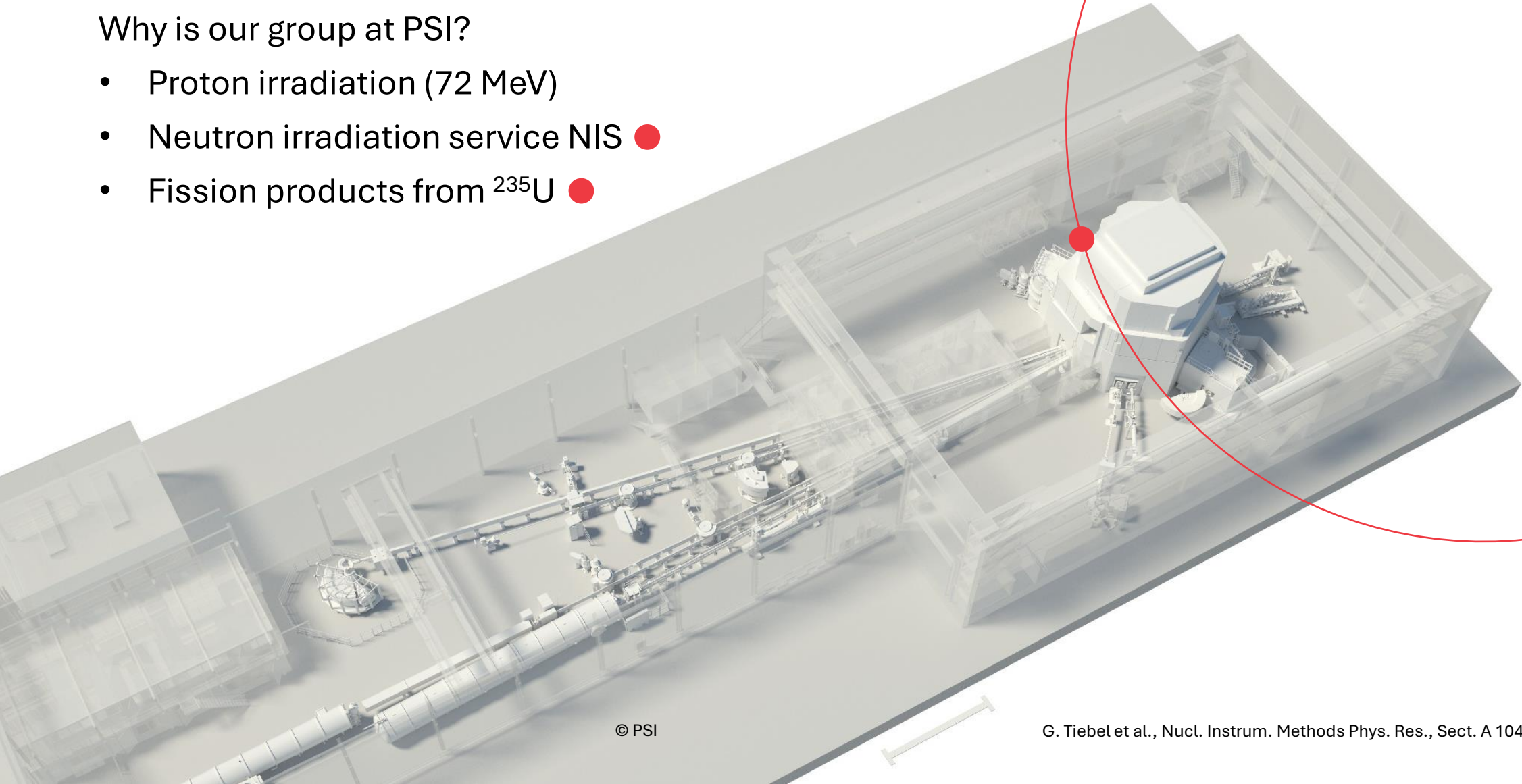


Tb 159 100	Tb 160 72.3 d β^- 0.6, 1.7... γ 879, 299 966... σ 23.8	Tb 161 6.89 d β^- 0.5... γ 26, 49, 75... e^-	Tb 162 7.76 m β^- 1.4, 2.4... γ 260, 808 888...	Tb 163 19.5 m β^- 0.8, 1.3... γ 351, 390 494...
Gd 158 24.84	Gd 159 18.479 h β^- 1.0... γ 364, 58...	Gd 160 21.86 σ 1.4	Gd 161 5.66 m β^- 1.1, 1.7... γ 361, 315 102... σ 19000	Gd 162 8.2 m β^- 1.0... γ 442, 403...

Radionuclide Production at PSI

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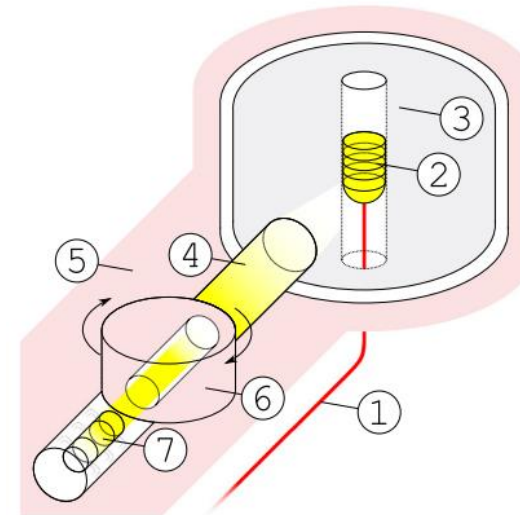
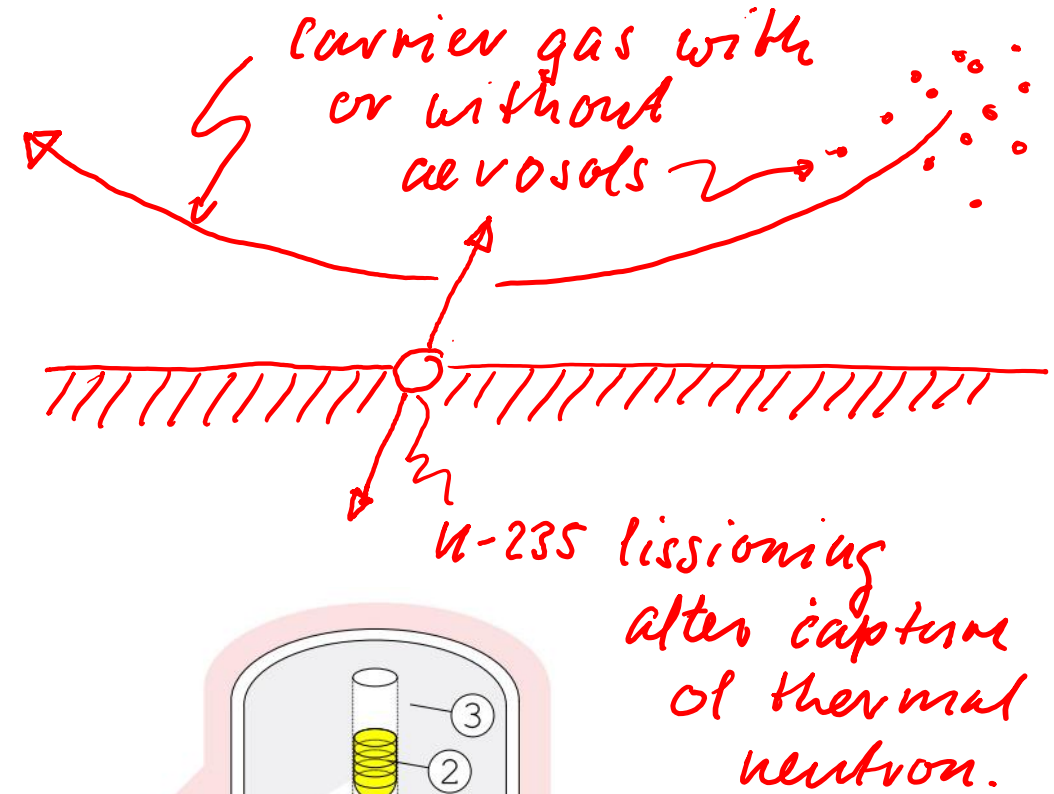
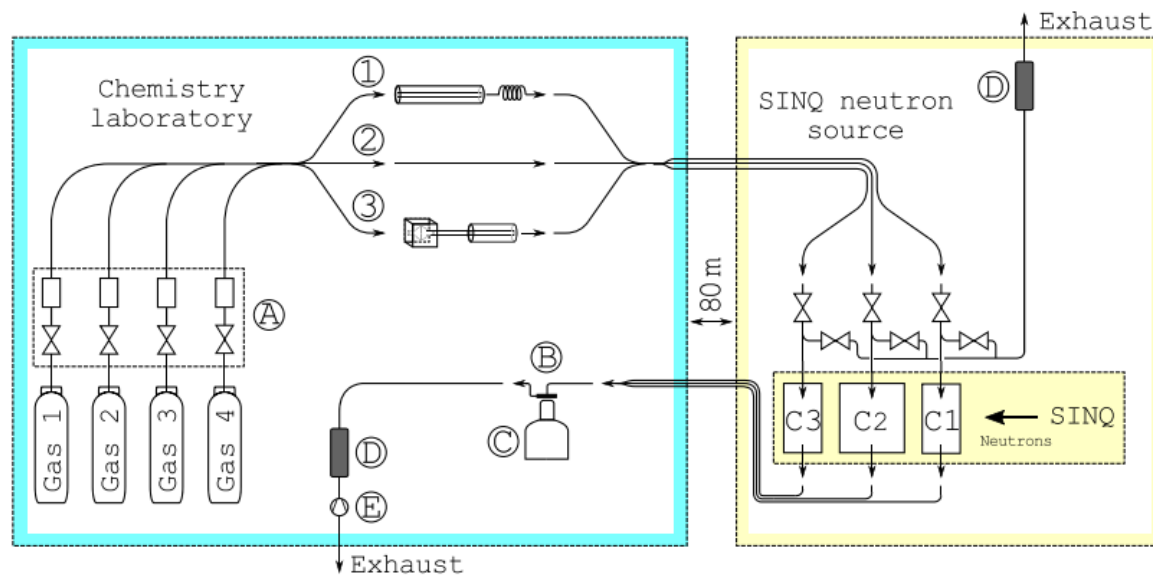
- Proton irradiation (72 MeV)
- Neutron irradiation service NIS ●
- Fission products from ^{235}U ●



Radionuclide Production at PSI

Thermal neutron-induced fission of ^{235}U

- **Volatile fission products** transported with a suitable carrier gas (e.g., N_2 or Ar).
- **Non-volatile fission products** transported with a aerosol-loaded (e.g., KCl) carrier gas.

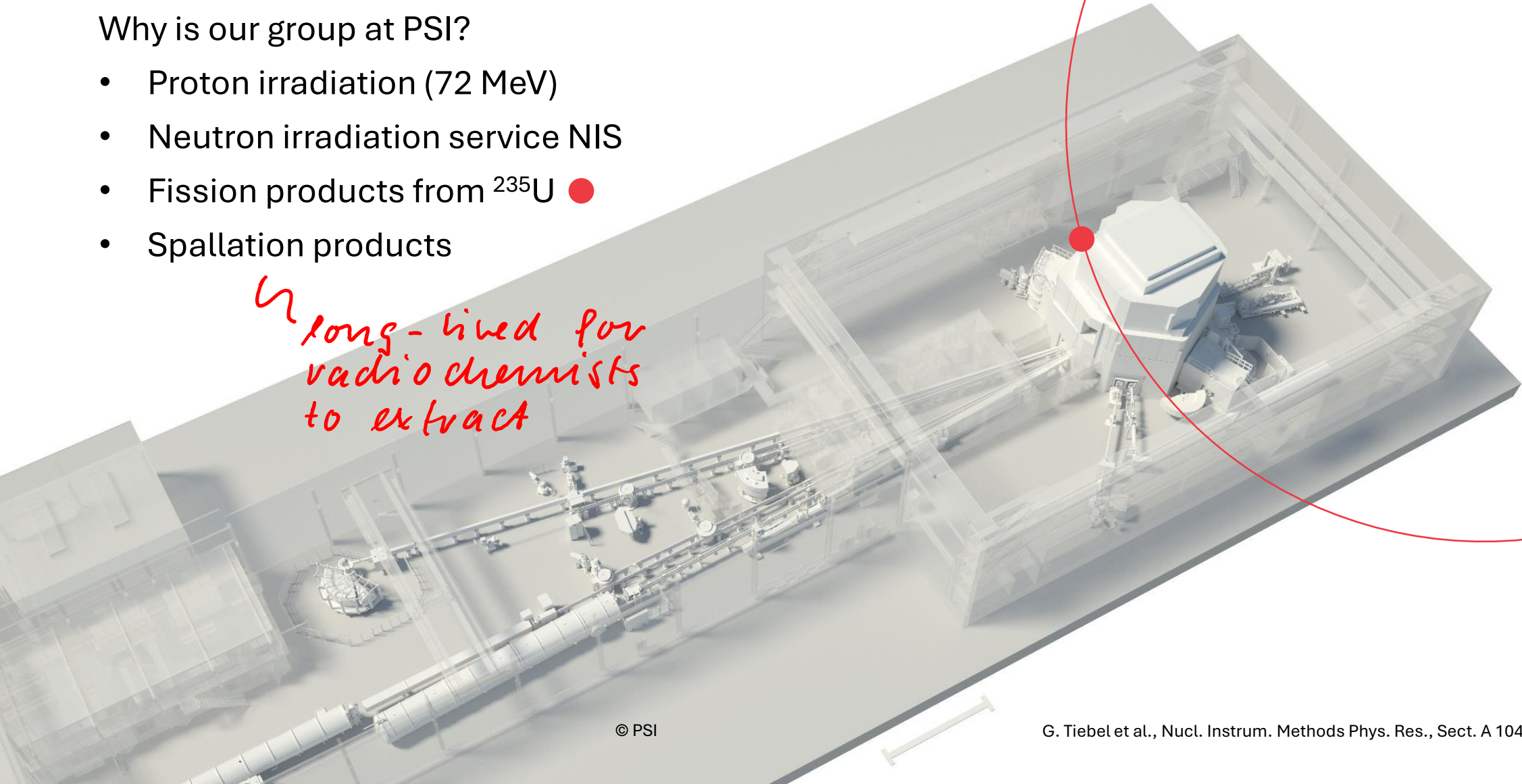


Radionuclide Production at PSI

Why is our group at PSI?

- Proton irradiation (72 MeV)
- Neutron irradiation service NIS
- Fission products from ^{235}U ●
- Spallation products

↳ long-lived for radiochemists to extract



Chemistry Experiments with Superheavy Elements



250.000 €

What name was given to the chemical element with atomic number 110 in 2003?

A Darmstadtium

B Bonnum

C Oldenburgium

D Frankfurtium



250.000 €

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57 La lanthanum 138.91 ± 0.01	58 Ce cerium 140.12 ± 0.01	59 Pr praseodymium 140.91 ± 0.01	60 Nd neodymium 144.24 ± 0.01	61 Pm promethium [145]	62 Sm samarium 150.36 ± 0.02	63 Eu europium 151.96 ± 0.01	64 Gd gadolinium 157.25 ± 0.03	65 Tb terbium 158.93 ± 0.01	66 Dy dysprosium 162.50 ± 0.01	67 Ho holmium 164.93 ± 0.01	68 Er erbium 167.26 ± 0.01	69 Tm thulium 168.93 ± 0.01	70 Yb ytterbium 173.05 ± 0.02	71 Lu lutetium 174.97 ± 0.01
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Relativistic effects

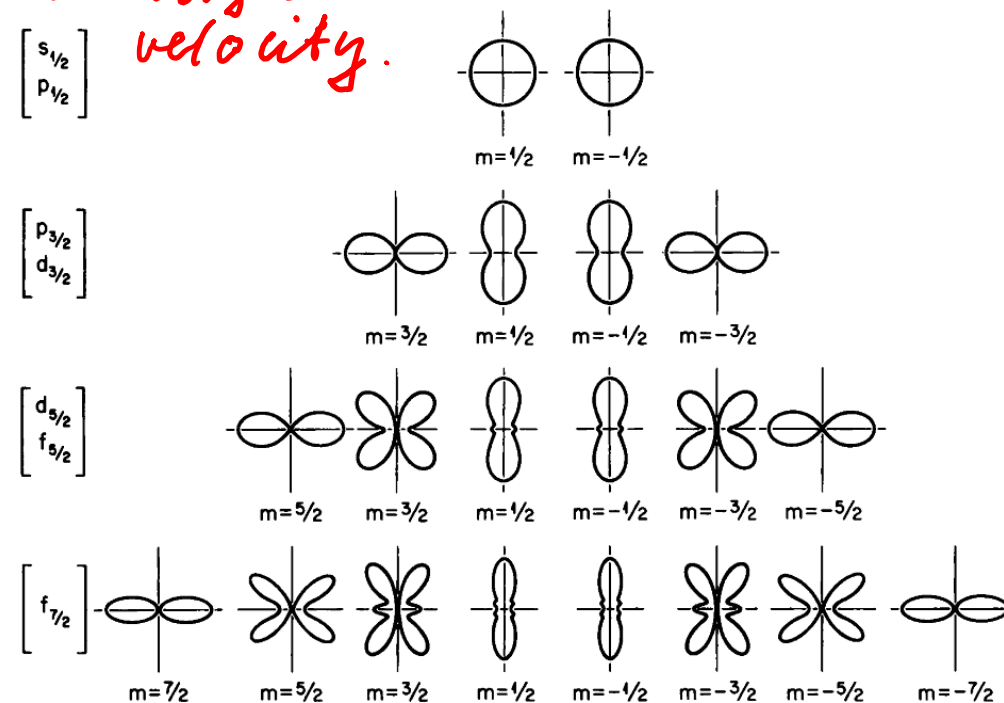
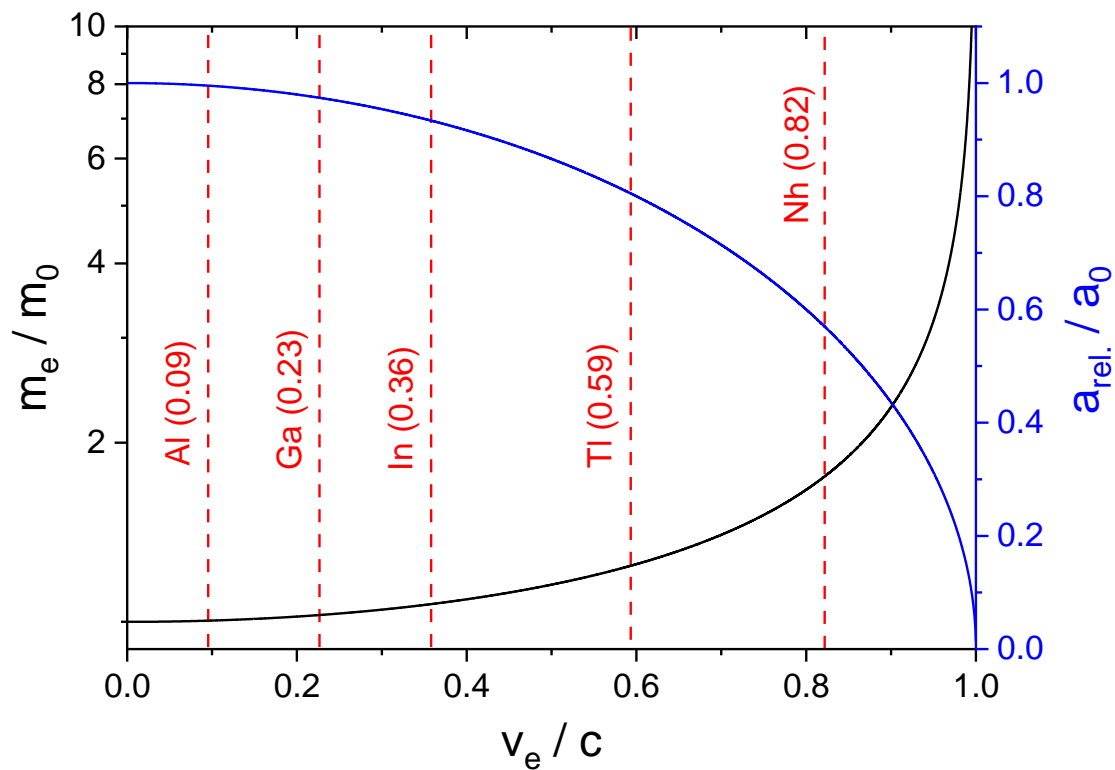
$$E = mc^2$$

Group 13 of the periodic table and the influences of relativistic effects (*ns*-Orbitals).

$$m_e = \frac{m_0}{\sqrt{1 - \left(\frac{v_e}{c}\right)^2}}$$

$$a_0 = n^2 \cdot \frac{4 \cdot \pi \cdot \epsilon_0 \cdot \hbar^2}{Z^2 \cdot m_e \cdot e^2}$$

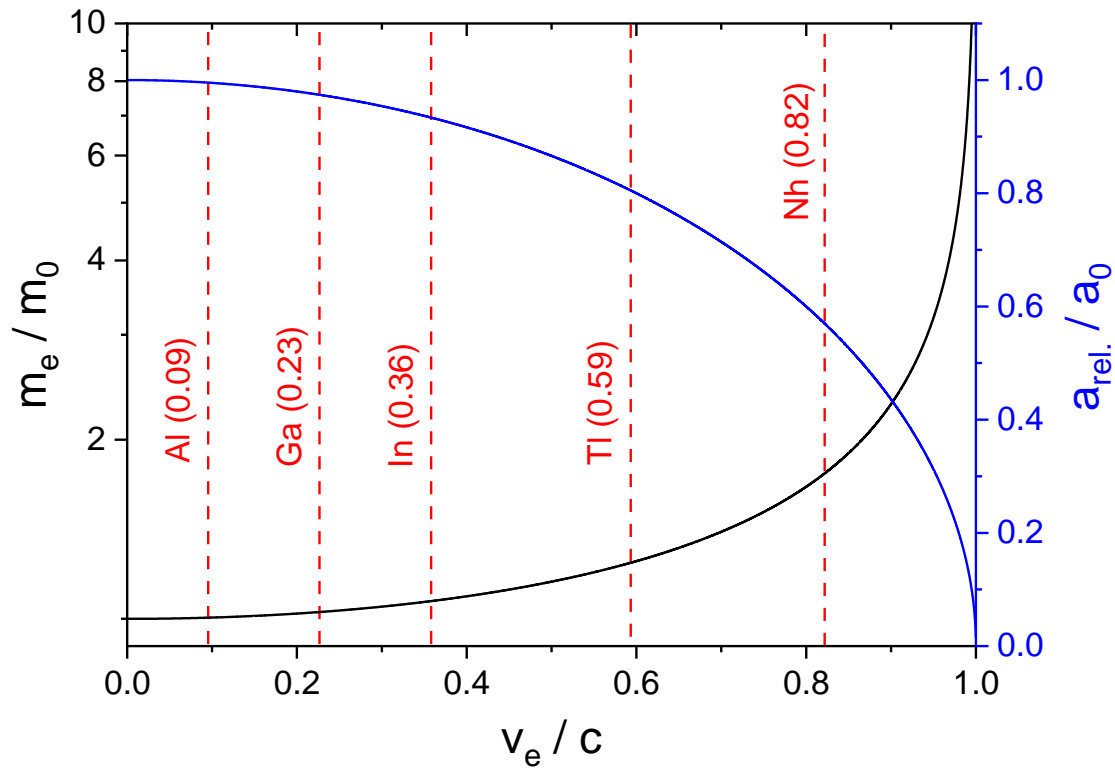
electron "gains" mass due to its higher velocity.



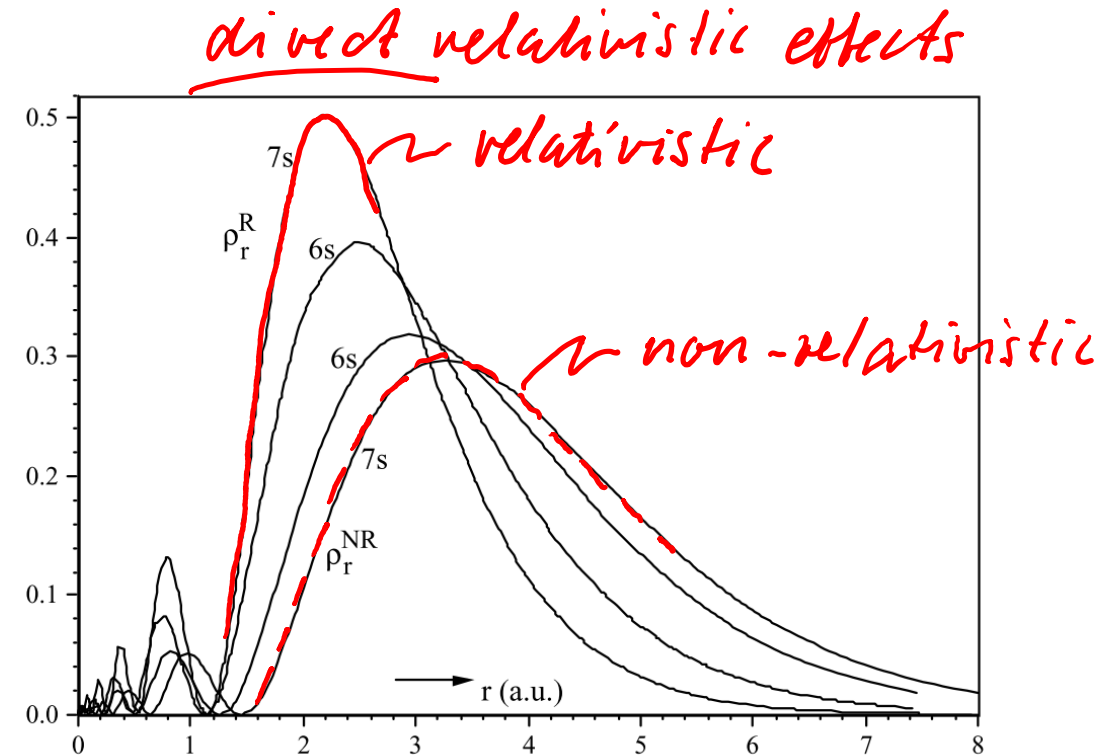
[Adapted from H. E. White, Phys. Rev. (1931)]

Relativistic effects

Group 13 of the periodic table and the influences of relativistic effects (ns-Orbitals).

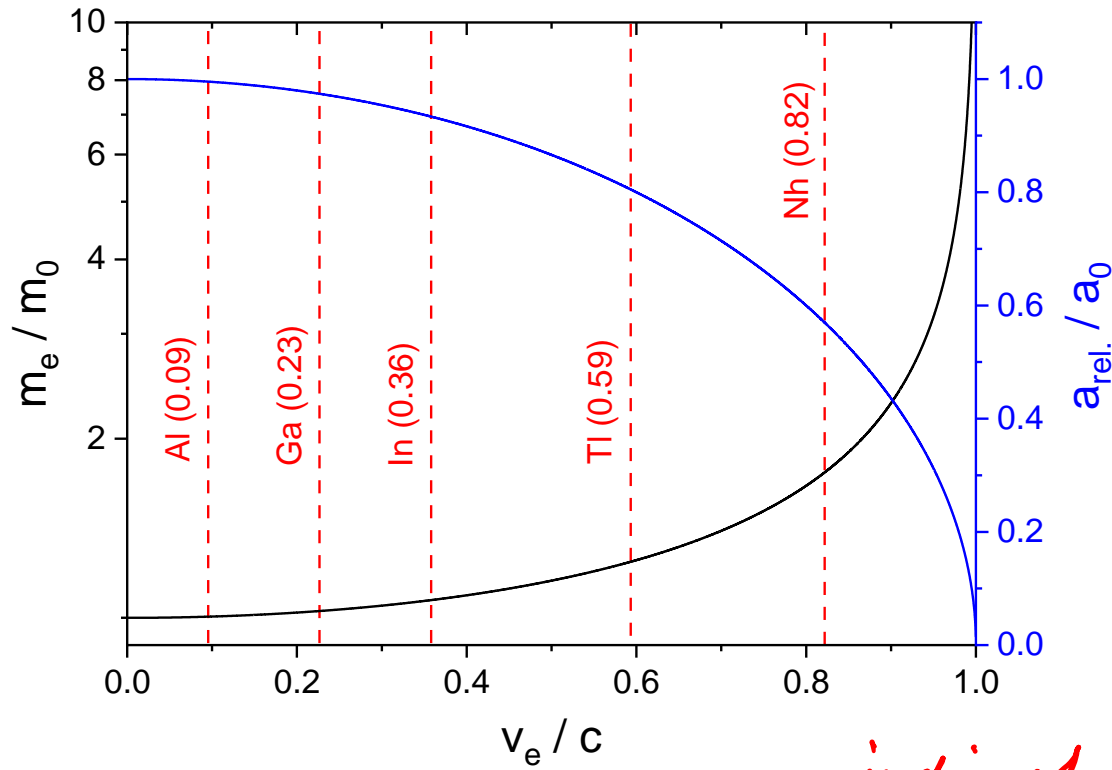


We differentiate between different relativistic effects; these are:

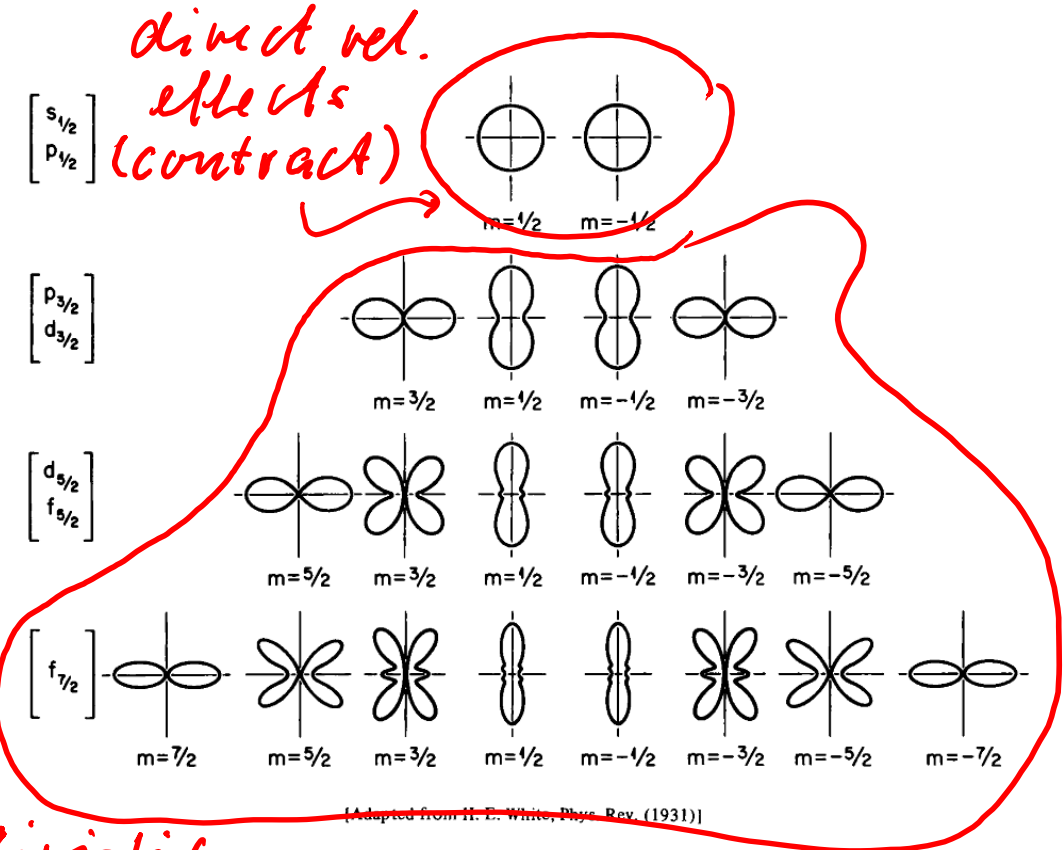


Relativistic effects

Group 13 of the periodic table and the influences of relativistic effects (ns-Orbitals).



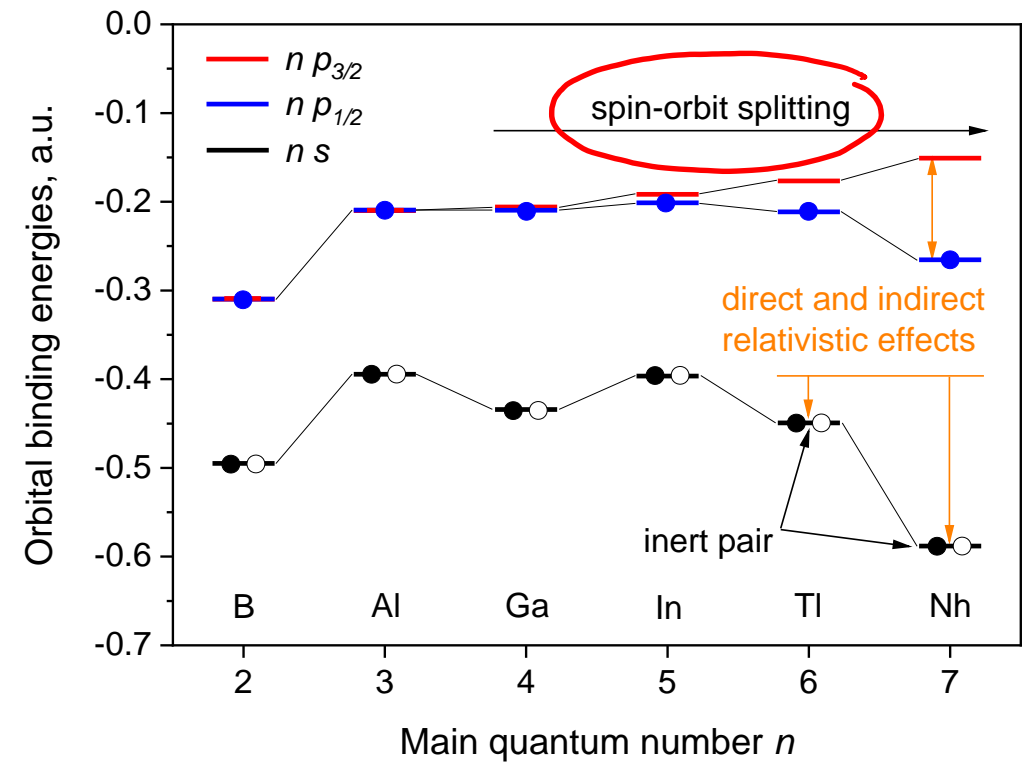
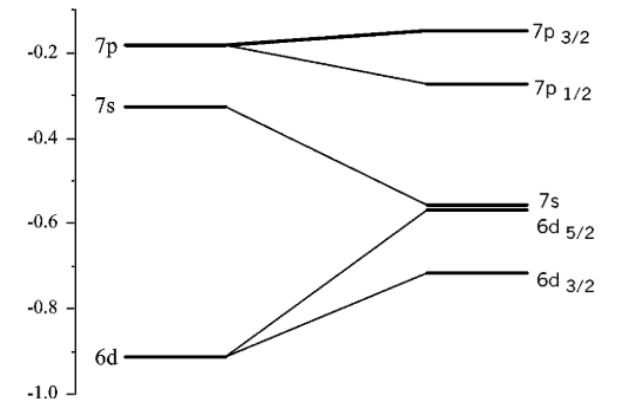
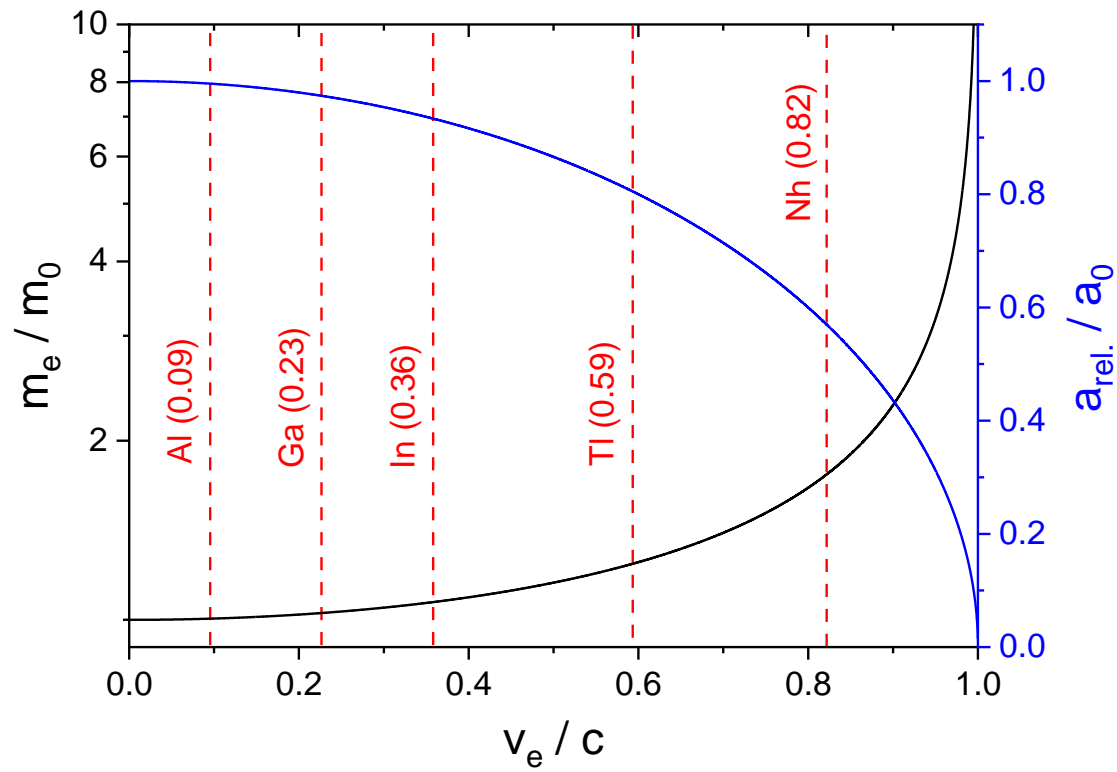
We differentiate between different relativistic effects; these are:



[Adapted from H. E. White, Phys. Rev. (1931)]

Relativistic effects

Group 13 of the periodic table and the influences of relativistic effects (ns-Orbitals).



Where else?

PRL 106, 018301 (2011)

PHYSICAL REVIEW LETTERS

week ending
7 JANUARY 2011

Relativity and the Lead-Acid Battery

Rajeev Ahuja,^{1,*} Andreas Blomqvist,¹ Peter Larsson,¹ Pekka Pyykkö,^{2,†} and Patryk Zaleski-Ejgierd^{2,‡}

¹Division of Materials Theory, Department of Physics and Astronomy, Uppsala University, Box 516, SE-751 20, Uppsala, Sweden

²Department of Chemistry, University of Helsinki, Box 55 (A.I. Virtasen aukio 1), FI-00014 Helsinki, Finland

(Received 30 August 2010; published 5 January 2011)

The energies of the solid reactants in the lead-acid battery are calculated *ab initio* using two different basis sets at nonrelativistic, scalar-relativistic, and fully relativistic levels, and using several exchange-correlation potentials. The average calculated standard voltage is 2.13 V, compared with the experimental value of 2.11 V. All calculations agree in that 1.7–1.8 V of this standard voltage arise from relativistic effects, mainly from PbO₂ but also from PbSO₄.

DOI: 10.1103/PhysRevLett.106.018301

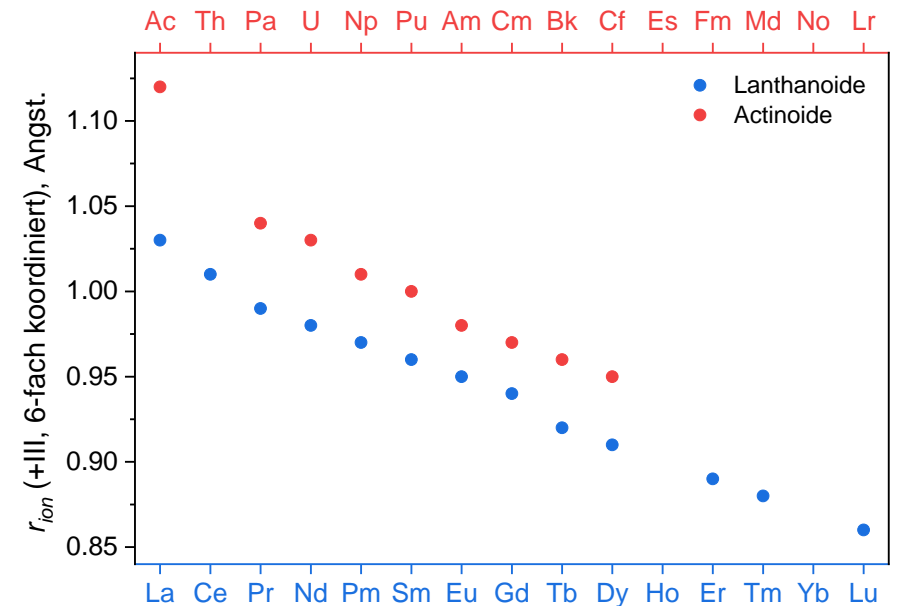
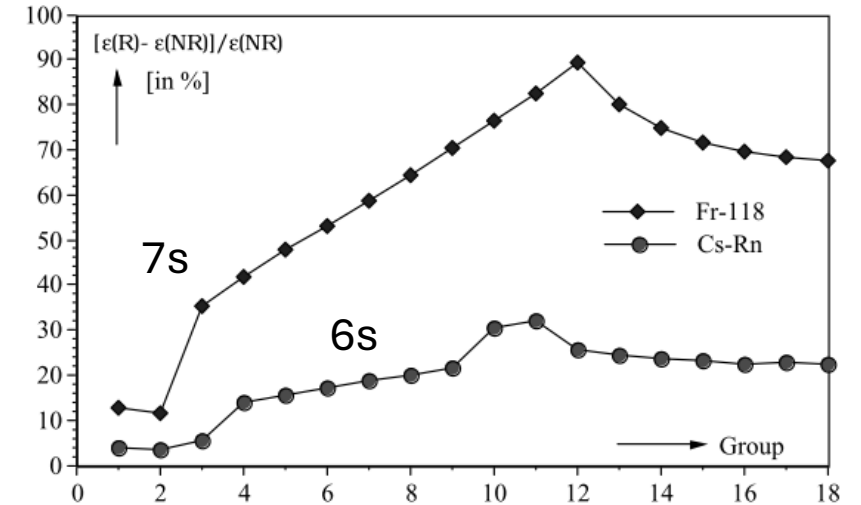
PACS numbers: 82.47.Cb, 31.15.ae, 31.15.aj, 82.60.Cx

Why Is Mercury Liquid?

Or, Why Do Relativistic Effects Not Get into Chemistry Textbooks?

Lars J. Norrby

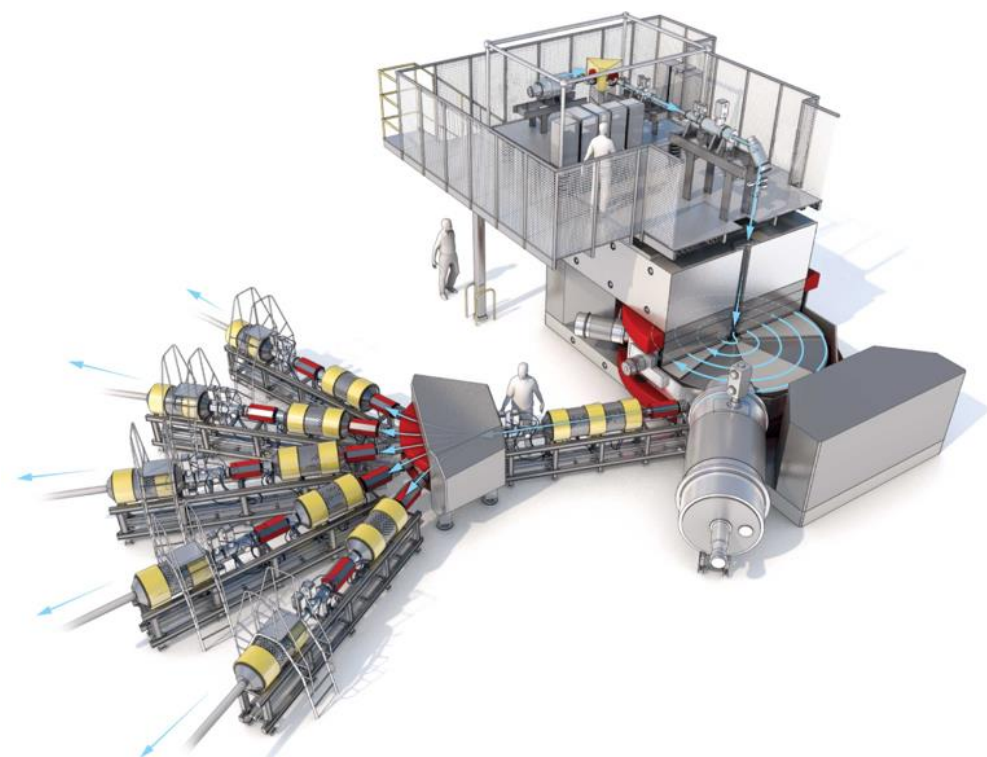
Royal Military College of Canada, Kingston, ON, Canada K7K 5L0





Chemical plant?

Fusion reactions.



The Alchemist's Cookbook

1 H hydrogen 1.0080 ± 0.0002																	18 He helium 4.0026 ± 0.0001						
3 Li lithium 6.94 ± 0.06	4 Be beryllium 9.0122 ± 0.0001																	13 B boron 10.81 ± 0.02	14 C carbon 12.011 ± 0.002	15 N nitrogen 14.007 ± 0.001	16 O oxygen 15.999 ± 0.001	17 F fluorine 18.998 ± 0.001	10 Ne neon 20.180 ± 0.001
11 Na sodium 22.990 ± 0.001	12 Mg magnesium 24.305 ± 0.002																	13 Al aluminium 26.982 ± 0.001	14 Si silicon 28.085 ± 0.001	15 P phosphorus 30.974 ± 0.001	16 S sulfur 32.06 ± 0.02	17 Cl chlorine 35.45 ± 0.01	18 Ar argon 39.95 ± 0.16
19 K potassium 39.098 ± 0.001	20 Ca calcium 40.078 ± 0.004	21 Sc scandium 44.956 ± 0.001	22 Ti titanium 47.867 ± 0.001	23 V vanadium 50.942 ± 0.001	24 Cr chromium 51.996 ± 0.001	25 Mn manganese 54.938 ± 0.001	26 Fe iron 55.845 ± 0.002	27 Co cobalt 58.933 ± 0.001	28 Ni nickel 58.693 ± 0.001	29 Cu copper 63.546 ± 0.003	30 Zn zinc 65.38 ± 0.02	31 Ga gallium 69.723 ± 0.001	32 Ge germanium 72.630 ± 0.008	33 As arsenic 74.922 ± 0.001	34 Se selenium 78.971 ± 0.008	35 Br bromine 79.904 ± 0.003	36 Kr krypton 83.798 ± 0.002						
37 Rb rubidium 85.468 ± 0.001	38 Sr strontium 87.62 ± 0.01	39 Y yttrium 88.906 ± 0.001	40 Zr zirconium 91.224 ± 0.002	41 Nb niobium 92.906 ± 0.001	42 Mo molybdenum 95.95 ± 0.01	43 Tc technetium [97]	44 Ru ruthenium 101.07 ± 0.02	45 Rh rhodium 102.91 ± 0.01	46 Pd palladium 106.42 ± 0.01	47 Ag silver 107.87 ± 0.01	48 Cd cadmium 112.41 ± 0.01	49 In indium 114.82 ± 0.01	50 Sn tin 118.71 ± 0.01	51 Sb antimony 121.76 ± 0.01	52 Te tellurium 127.60 ± 0.03	53 I iodine 126.90 ± 0.01	54 Xe xenon 131.29 ± 0.01						
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Key:
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$3 \cdot 10^{12} \text{ s}^{-1}$

$2 \cdot 10^{18} \text{ atoms/cm}^2$

Accelerator

Ca
20

Source

Am
95

Target

Atoms per day

Mc
115

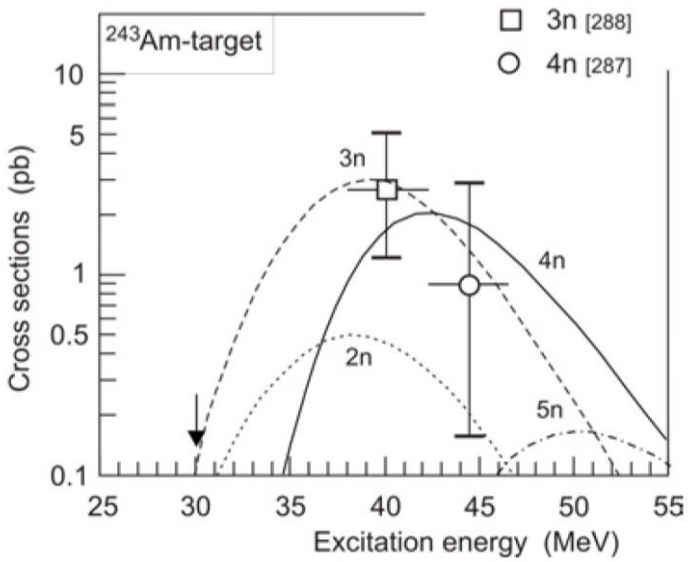
Physical
pre-separation

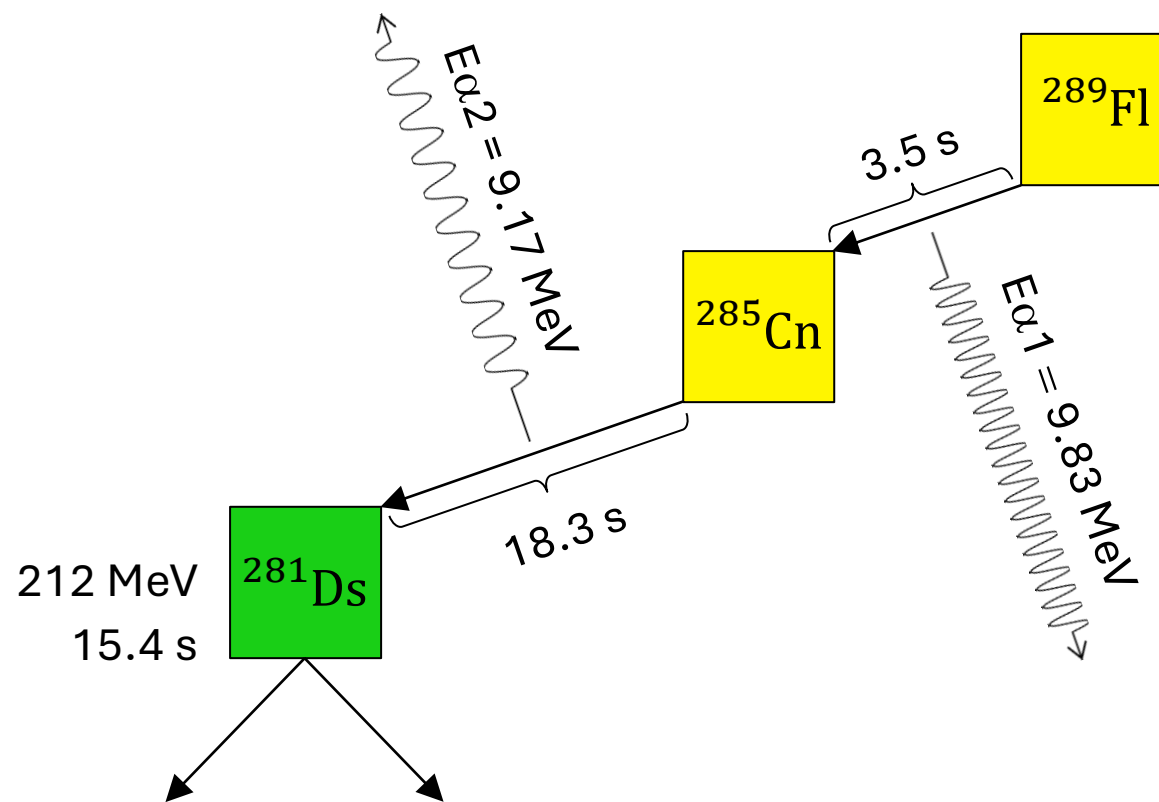
Coupling

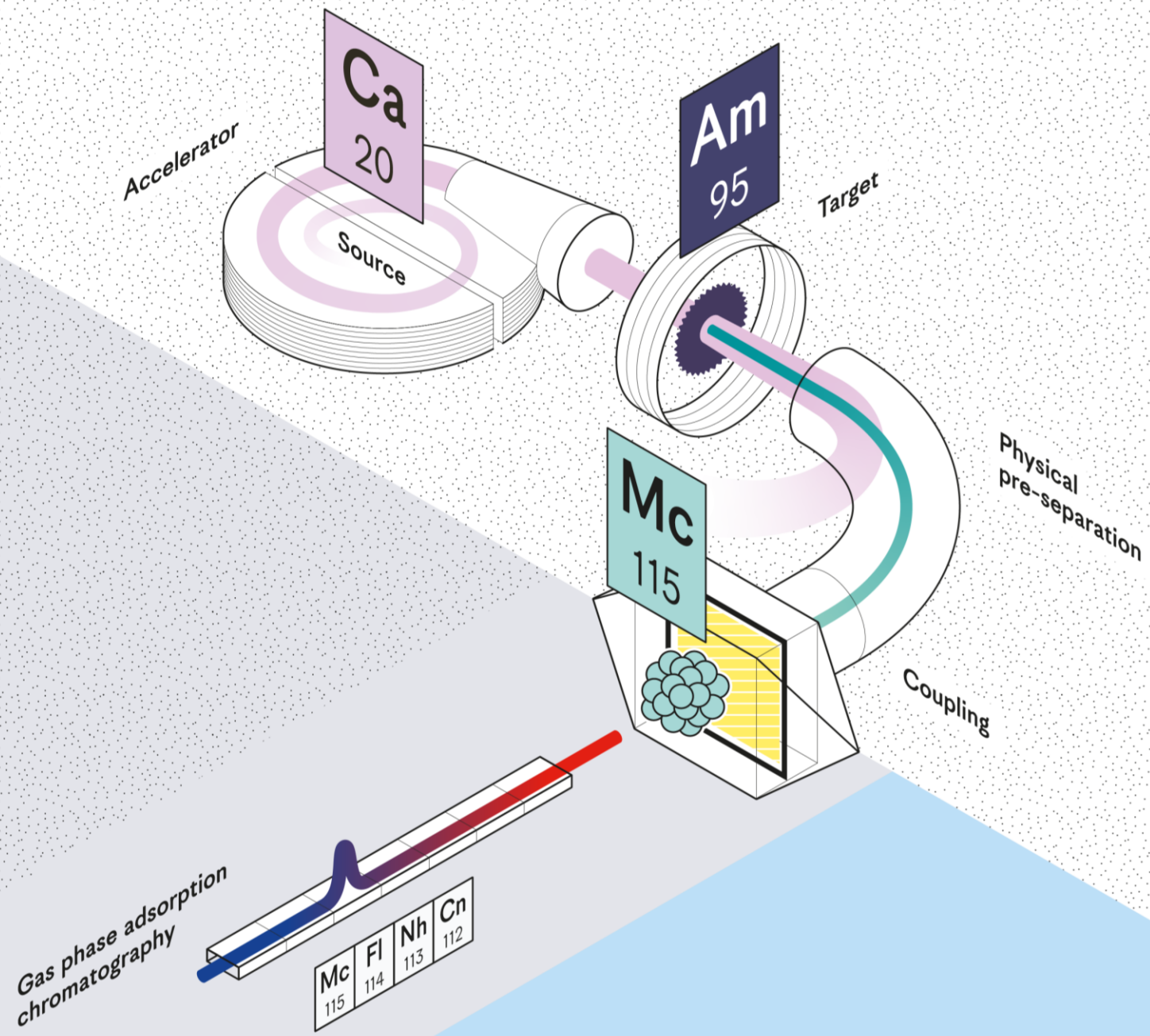
Physics world ($\geq \text{MeV}$)

Chemistry world ($< \text{eV}$)

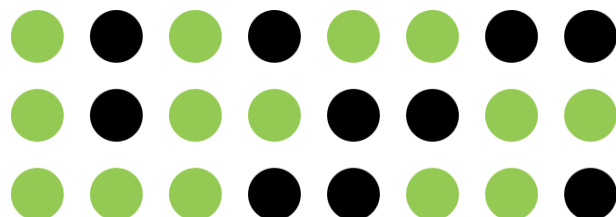
Nuclear reaction cross section



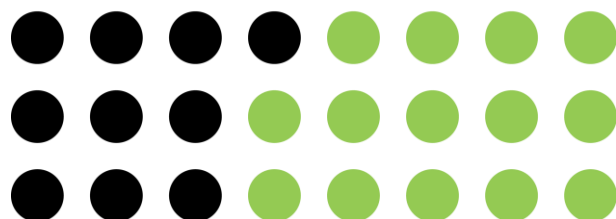




Classical Chemistry



X ATOMS, 1 STEP



K \rightarrow Concentrations

Chemistry with Superheavy Elements

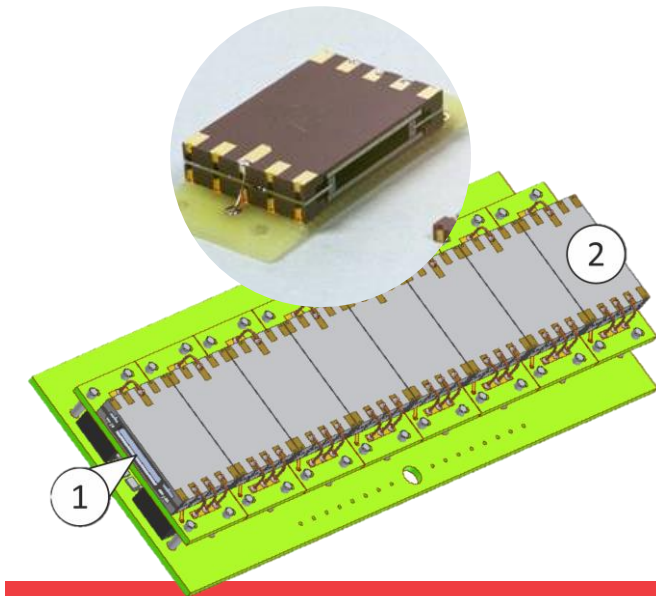
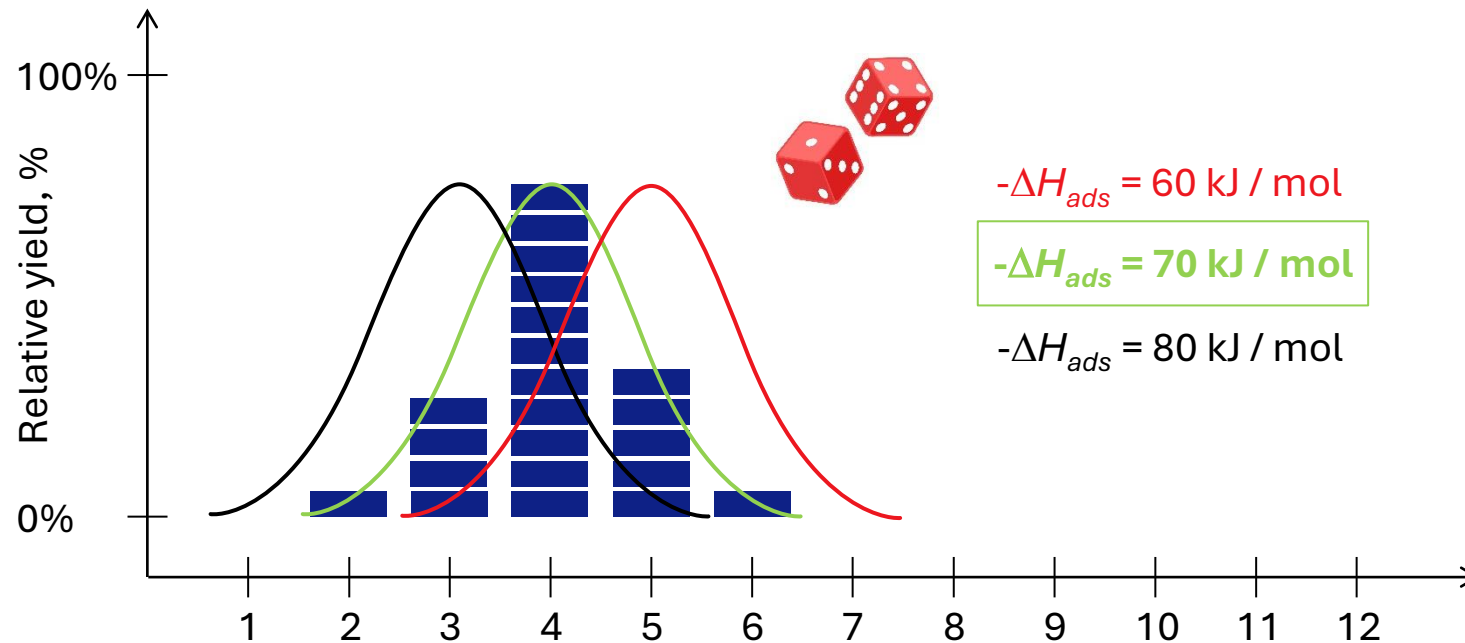
- Low production rates ($\approx 1 \text{ week}^{-1}$)
- Short life-times ($\approx 1 \text{ second}$)



K \rightarrow Probabilities

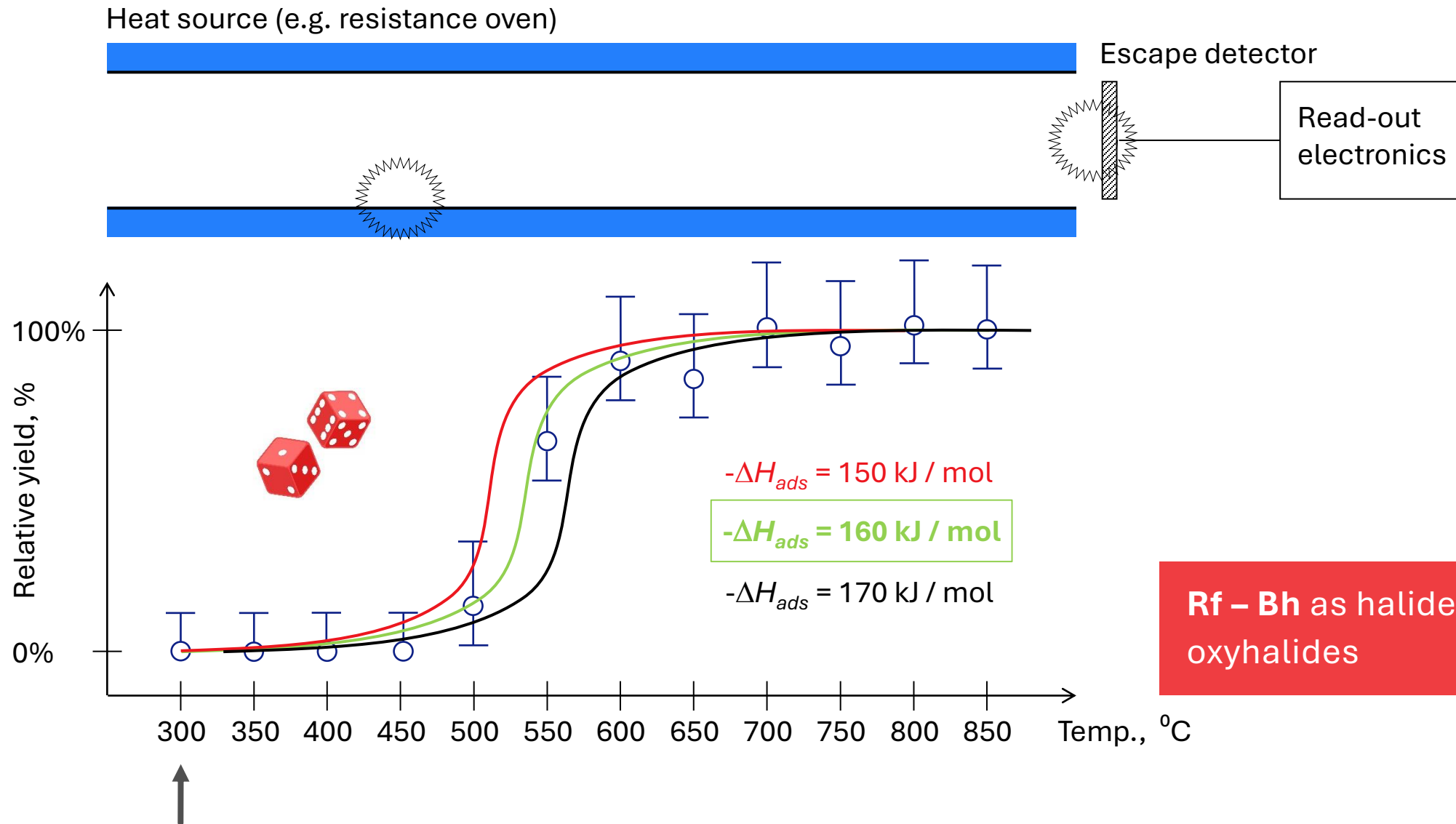
Thermochromatography

Negative temperature gradient

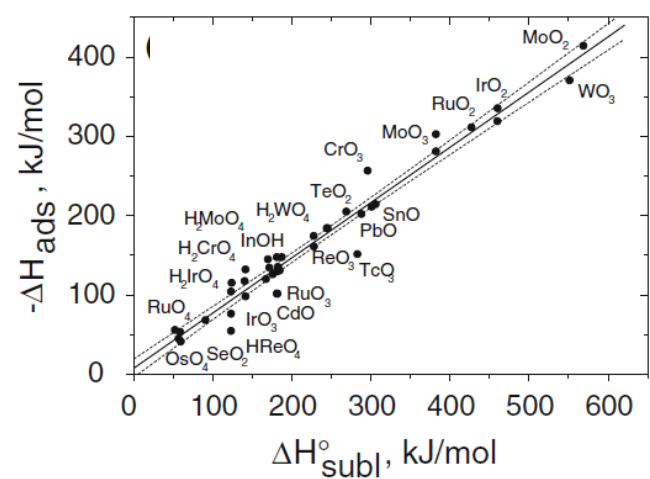
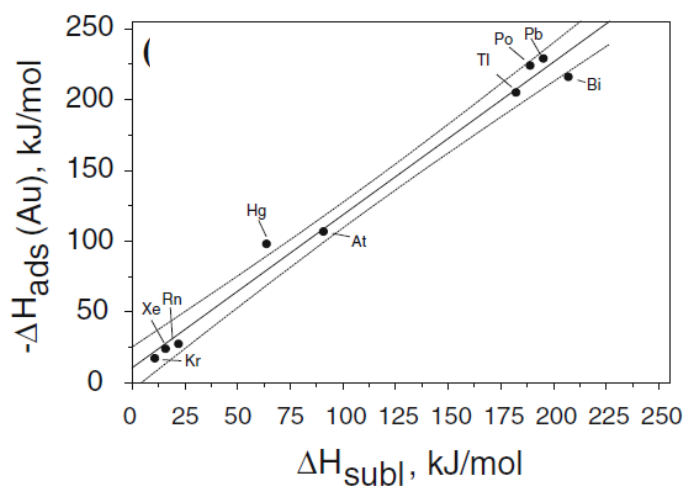
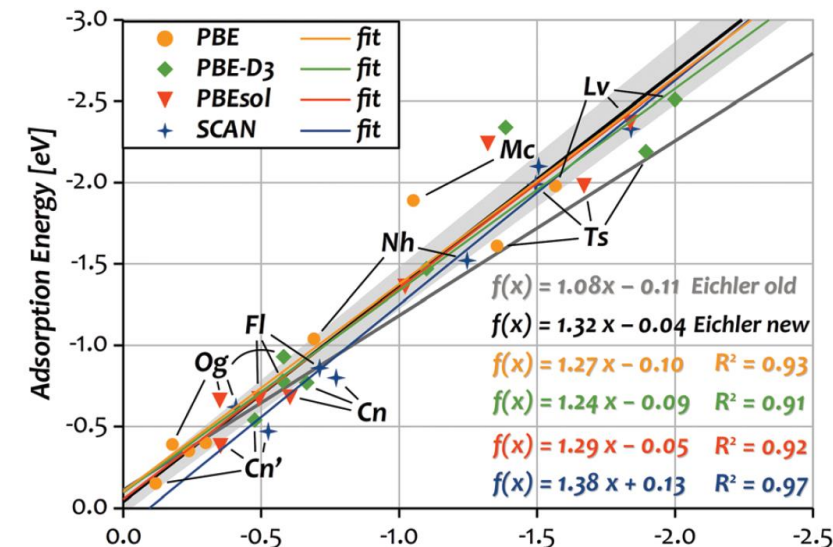
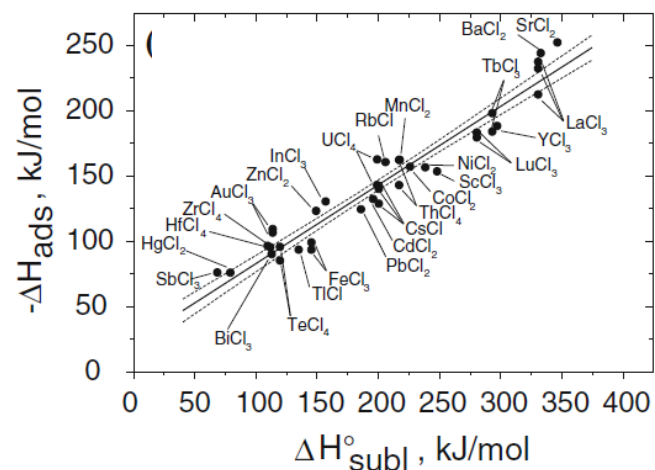
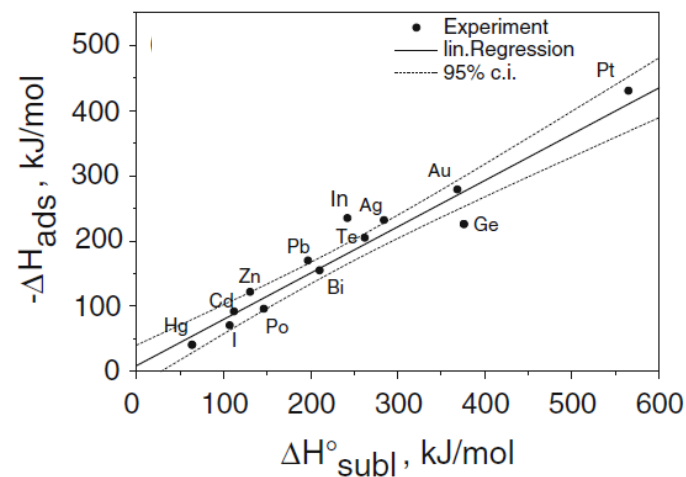


Rf – Hs as halides,
oxyhalides, and oxides + **Cn**,
Fl, and **Nh** (elemental?)

Isothermal chromatography

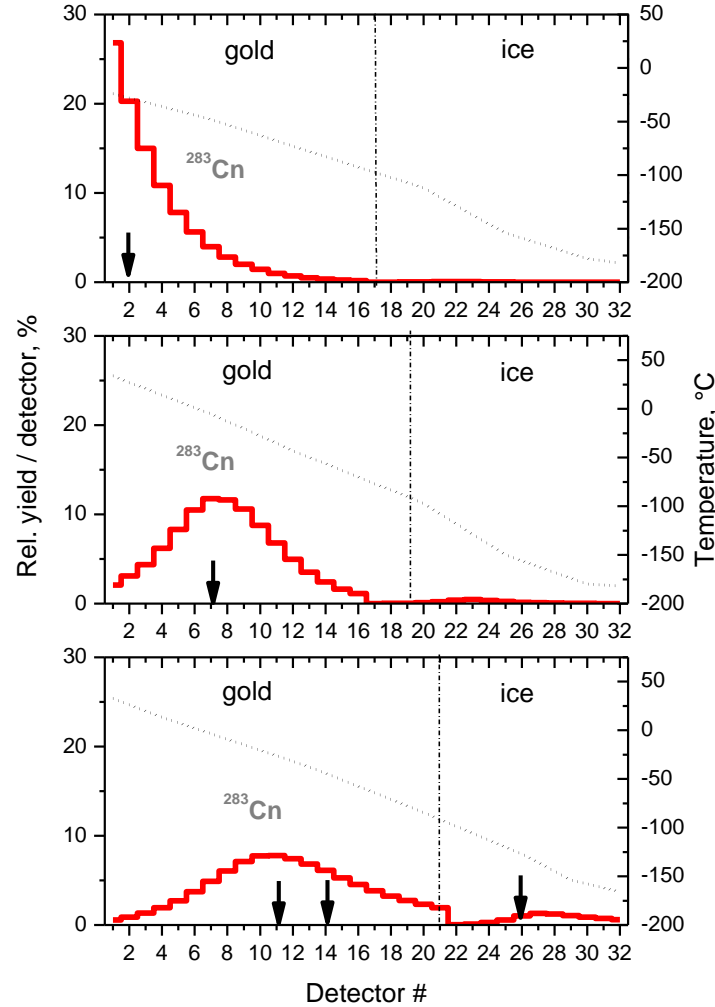
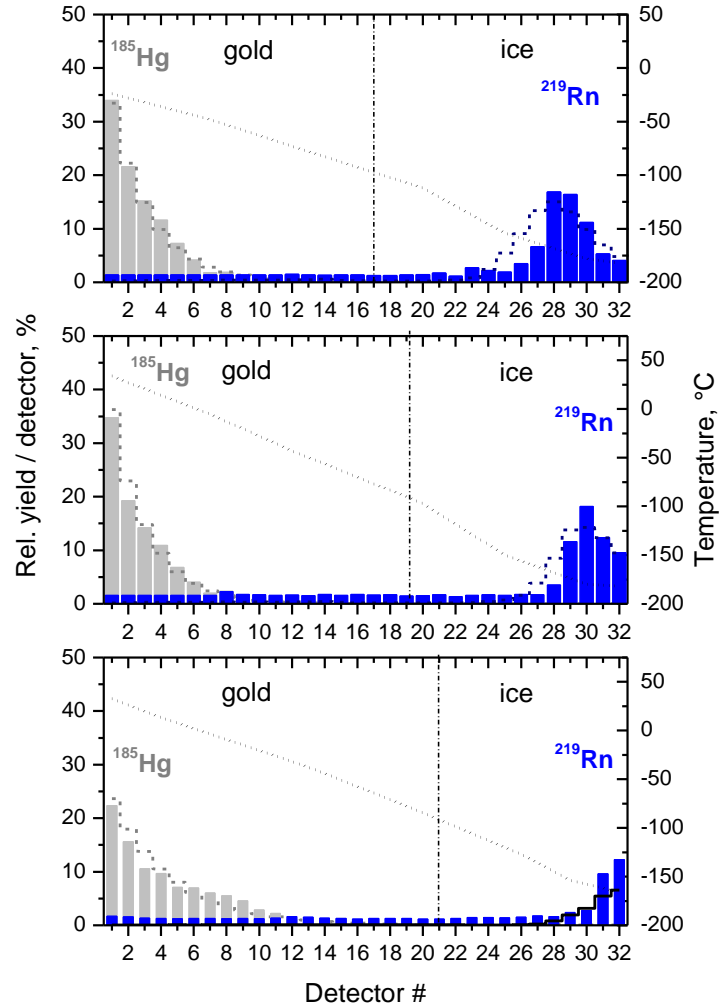


From single atoms to macroscopic amounts



Correlations include relativistic effects!

Example: Adsorption of Cn on Au



RESULTS (68% c.i.): Cn ($Z = 112$) is **very volatile** and, unlike Rn, reveals a **metallic interaction with Au** (typical group 12 element).

$$-\Delta H_{ads}^{Au}(\text{Cn}) = 52_{-3}^{+4} \text{ kJ/mol}$$

> How does this look with **nihonium** or a chemical compound of nihonium?

The Chemistry of Gen IV Nuclear Reactors

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3 Li lithium 6.94 ± 0.06	4 Be beryllium 9.0122 ± 0.0001																
11 Na sodium 22.990 ± 0.001	12 Mg magnesium 24.305 ± 0.002																
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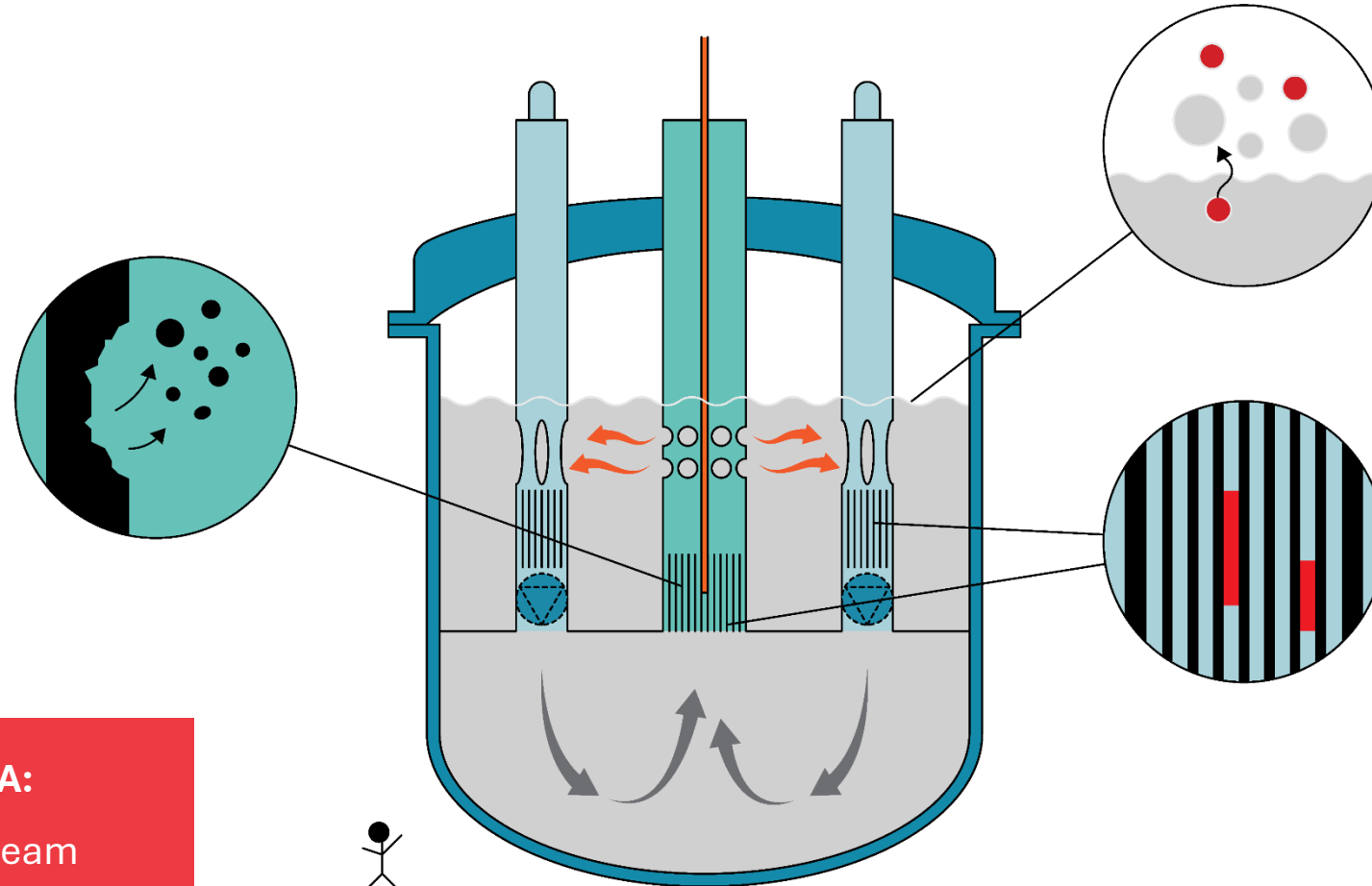


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The Chemistry of Gen IV Nuclear Reactors



Characteristics of MYRRHA:

- 600 MeV / 4 mA proton beam
- Sub-critical 65 – 100 MW_{th}
- LBE as coolant/spallation target

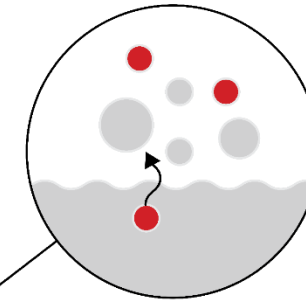
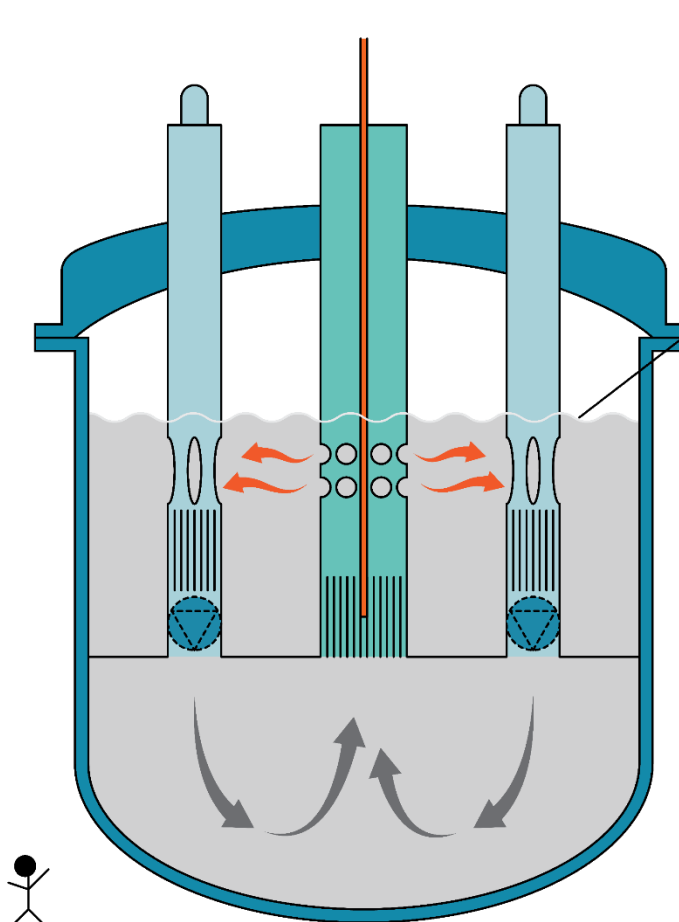
The Chemistry of Gen IV Nuclear Reactors

Main problem: Chemistry

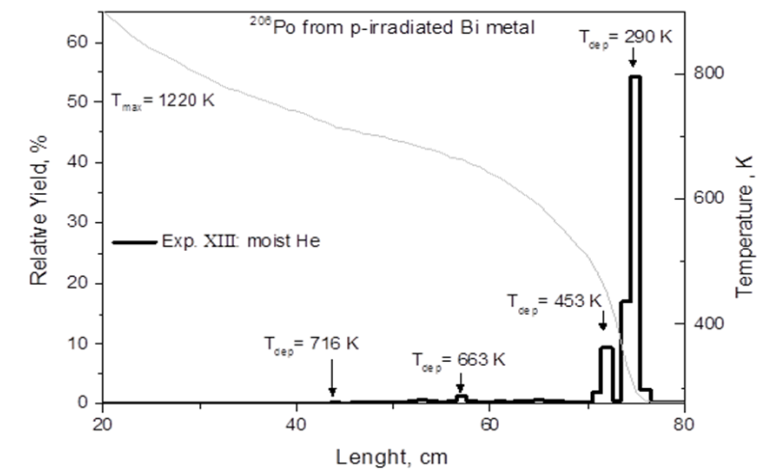
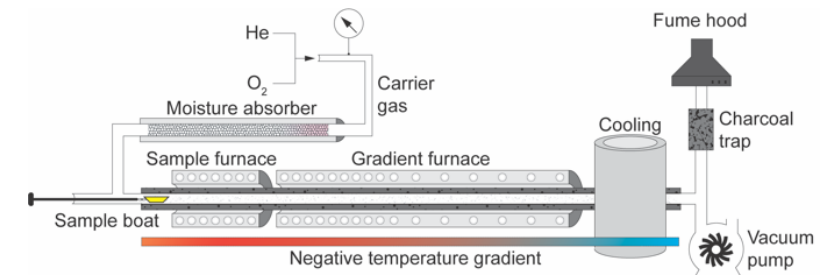
E.g., Po as large radiological risk

Characteristics:

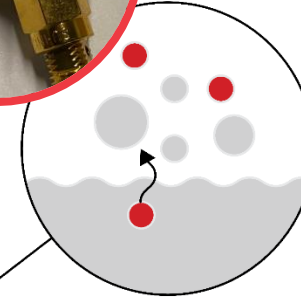
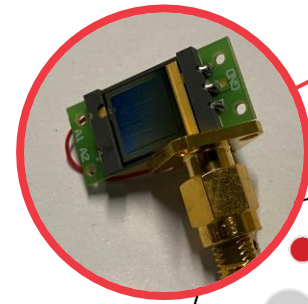
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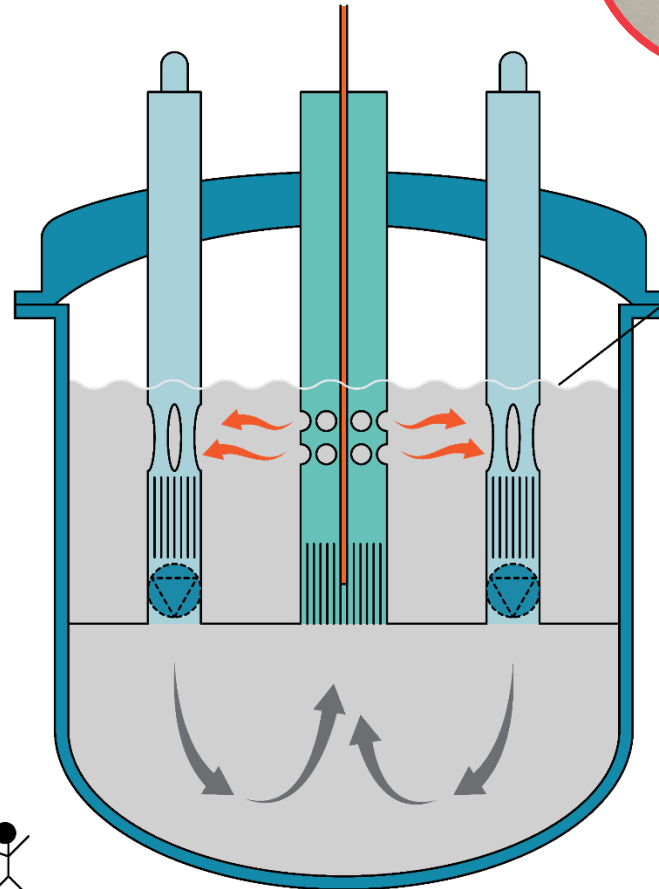
Same experimental gas-phase techniques as used for SHEs



The Chemistry of Gen IV Nuclear Reactors



Same experimental gas-phase techniques as used for SHEs

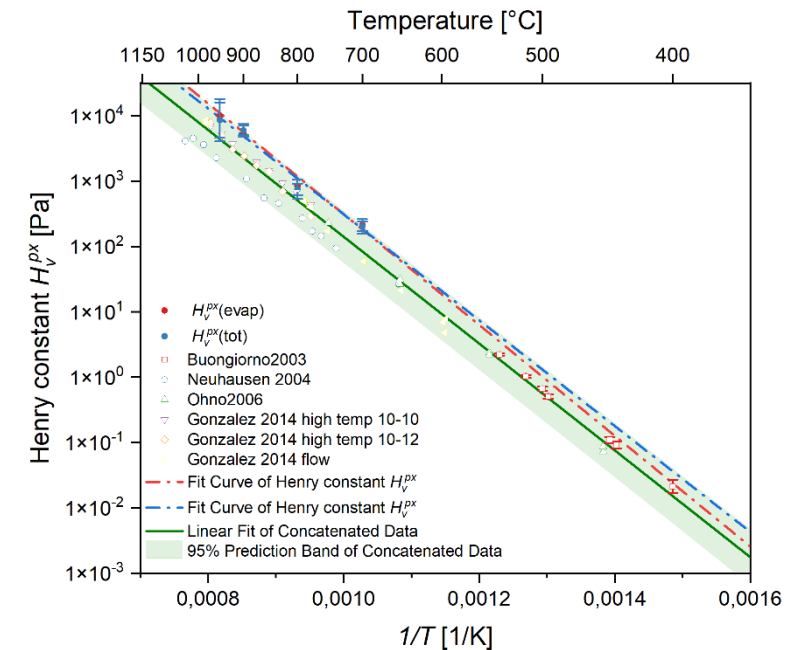


Main problem: Chemistry

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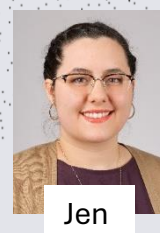
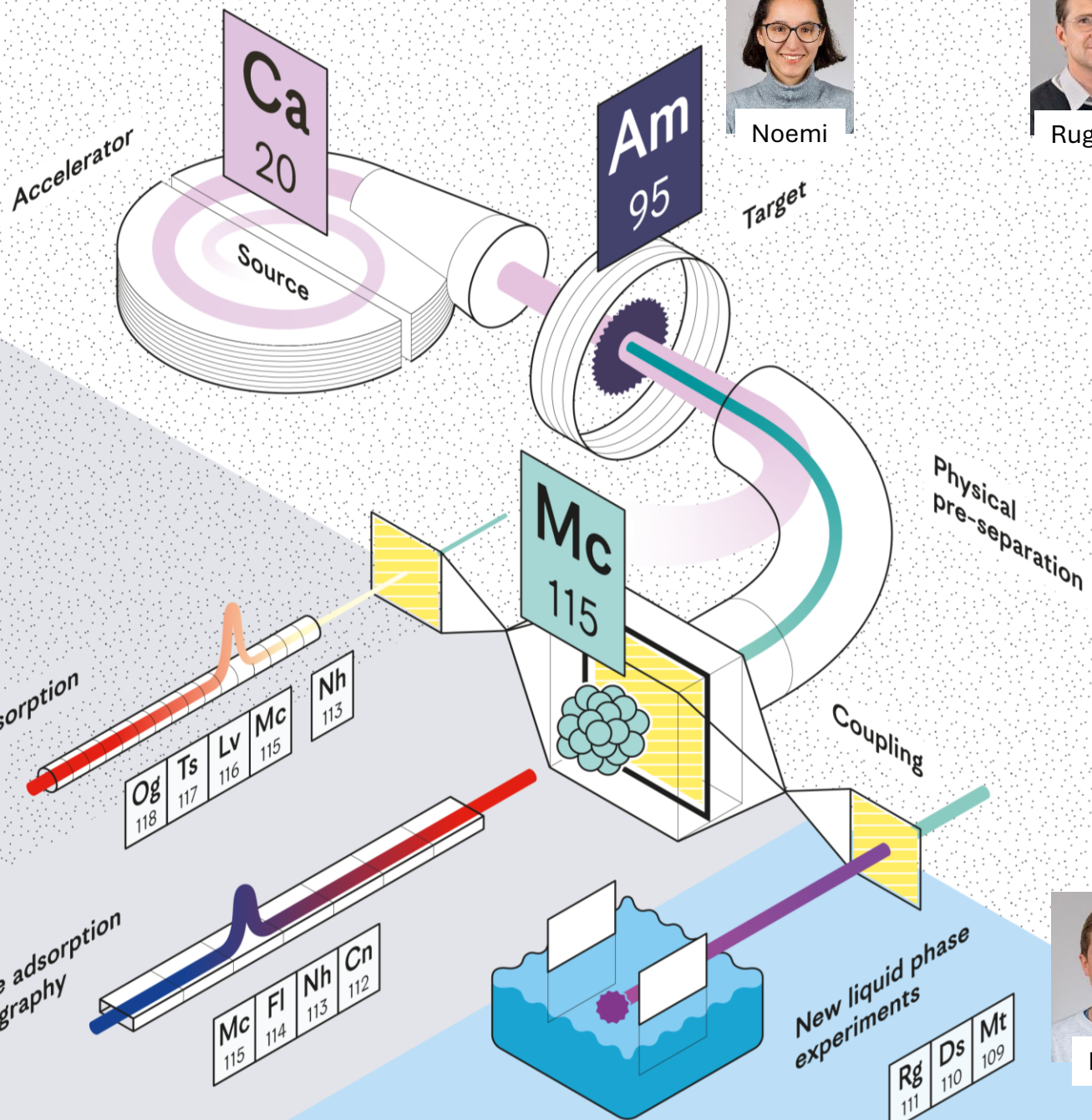


The end.

Superheavy elements


Swiss National Science Foundation


 Schweizerische Eidgenossenschaft
 Confédération suisse
 Confederazione Svizzera
 Confederaziun svizra





PSI Center for Nuclear Engineering
and Sciences



Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra



Swiss National
Science Foundation



Swiss Nanoscience Institute
Exzellenzzentrum
der Universität Basel und
des Kantons Aargau



中国科学院近代物理研究所
Institute of Modern Physics, Chinese Academy of Sciences



SENSIC

cividec
instrumentation



ETH zürich

PAUL SCHERRER INSTITUT



Video: <https://www.psi.ch/en/lrc/heavy-elements>