Bayesian uncertainty quantification for synthesizing superheavy elements

Seminar on 2025 July 2th

Source：Phys. Lett. B 858 (2024) 139069

In collaboration with Fang yueping, Zhu Long et. al.

LIAO ZeHong

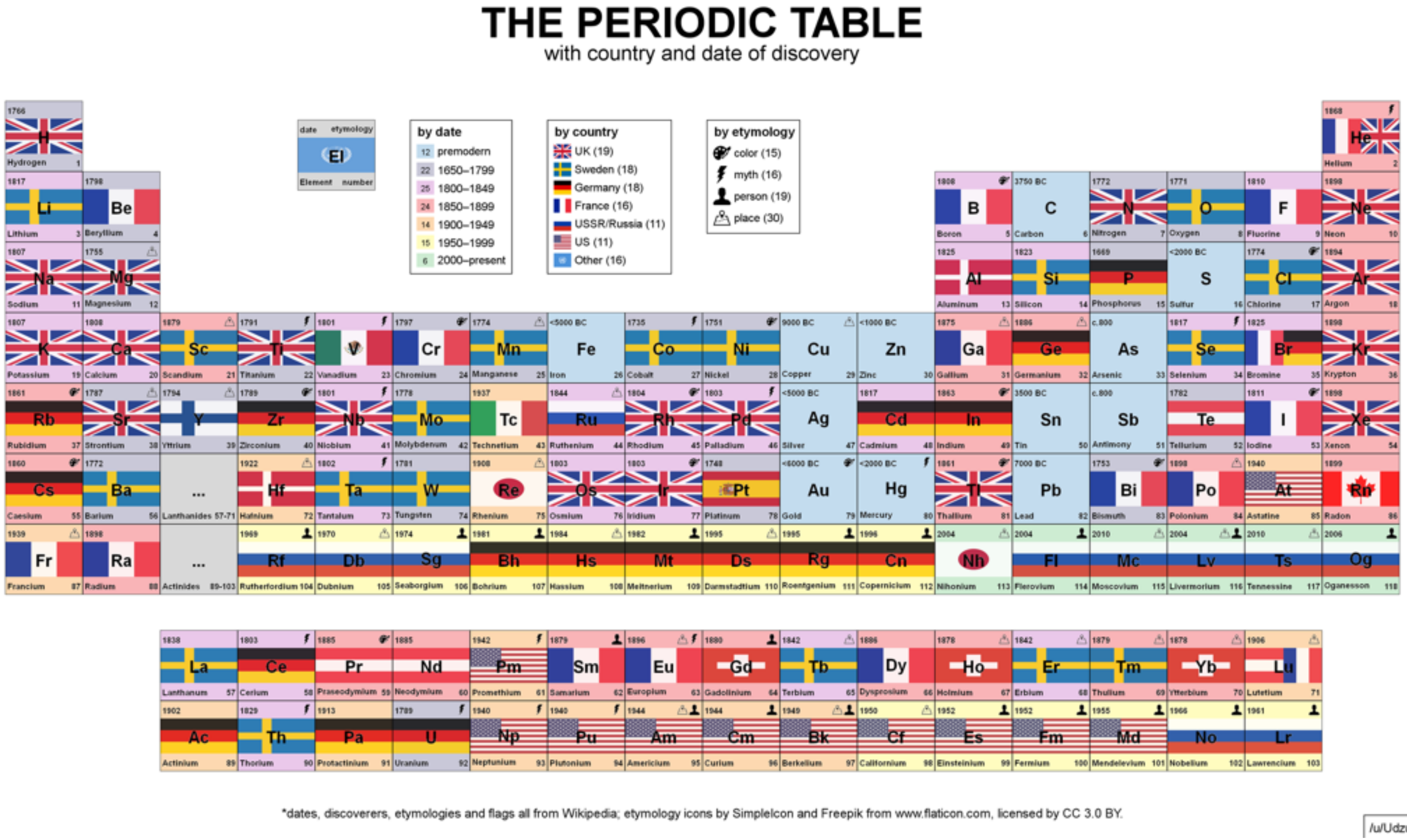
Sino-French Institute of Nuclear Engineering and Technology

The story began in this talk last year

Sino-French Institute of Nuclear Engineering and Technology

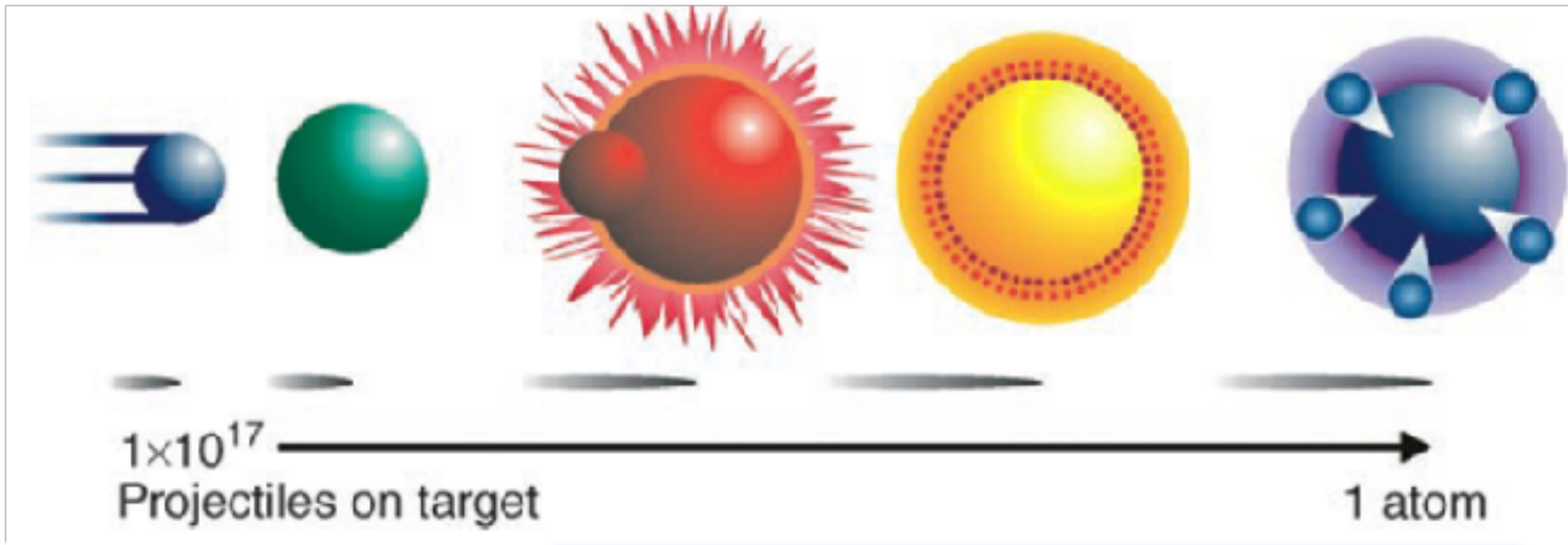
Content

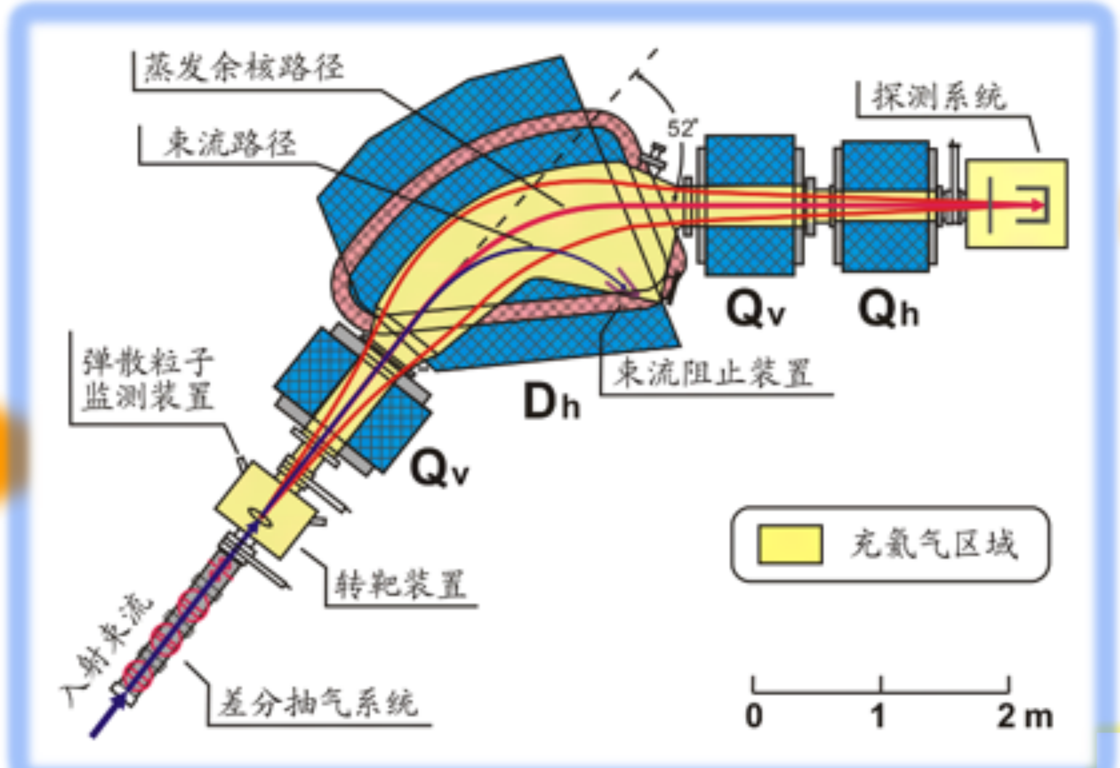
- The history of Superheavy element production
- The challenge of Superheavy element production
- Bayesian uncertainty quantification for synthesizing superheavy element

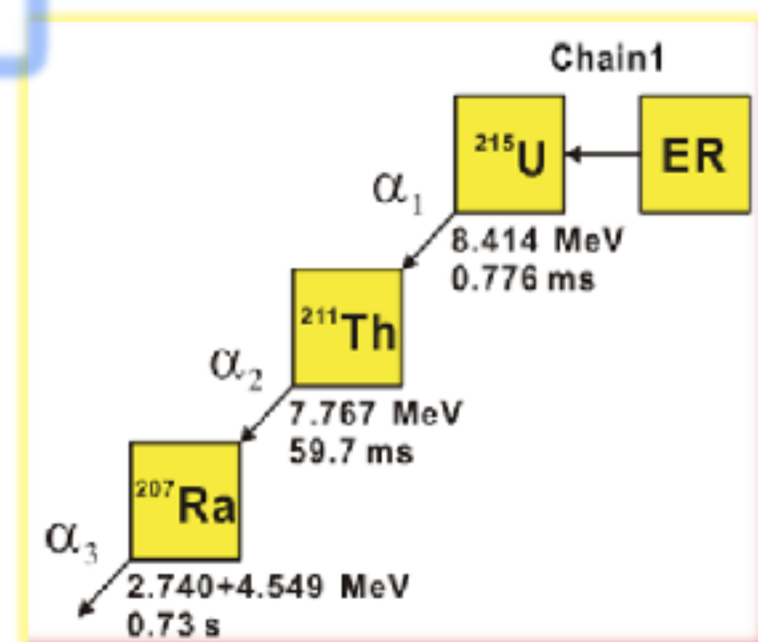


The only way we can create these elements is through nuclear reactions in the laboratory.

Fusion-evaporation reaction

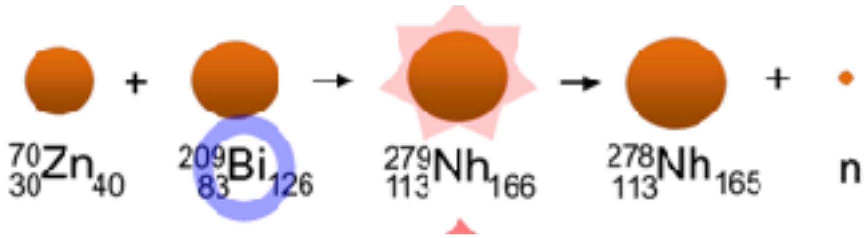






S. Hofmann, G. Münzenberg, Rev. Mod. Phys. 72 (2000) 733.

Cold fusion



GSI (Germany)

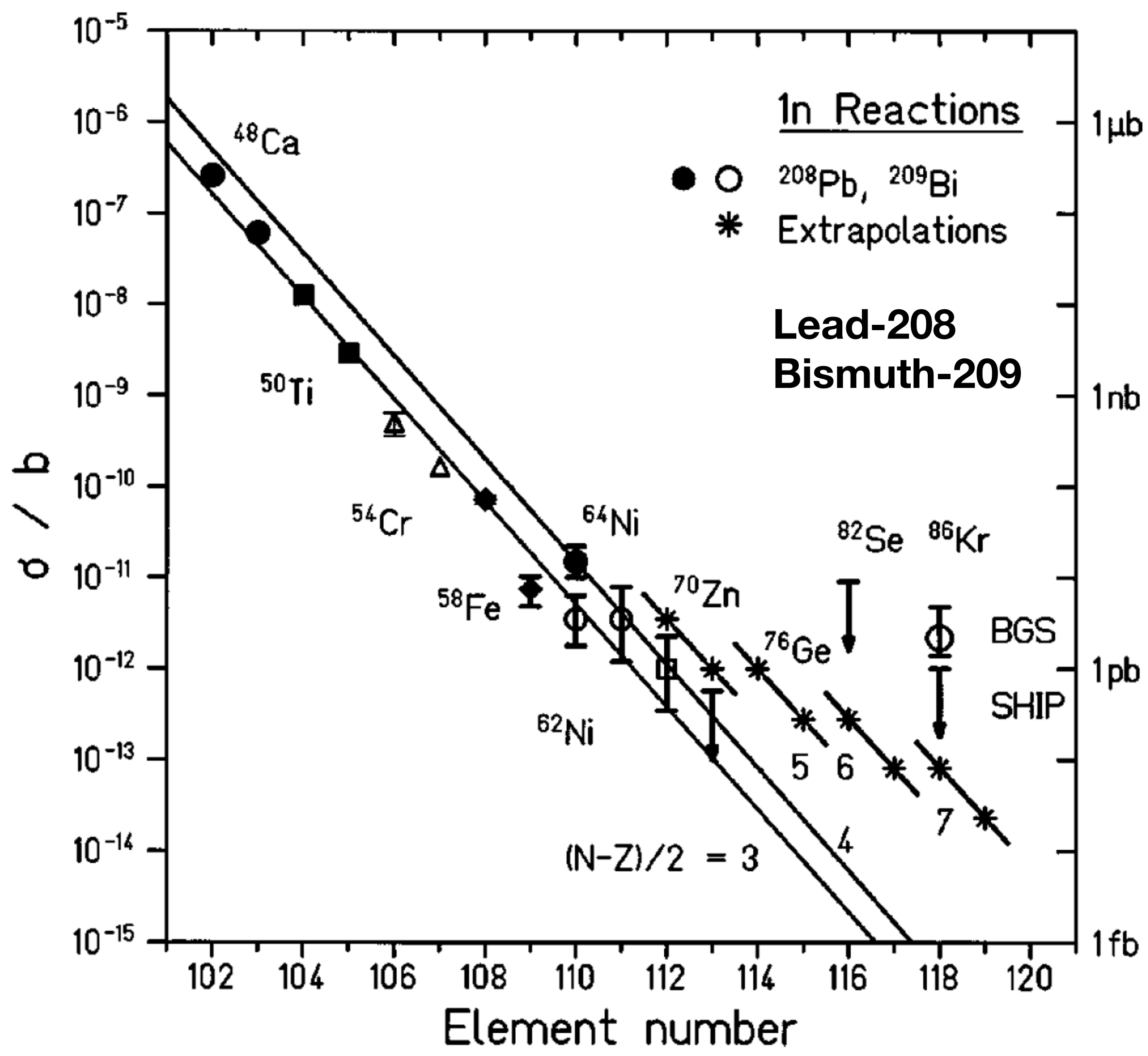
P. Armbruster

G. Münzenberg

S. Hofmann

Bh (107)
Hs (108)
Mt (109)
Ds (110)
Rg (111)
Cn (112)

Use ^{208}Pb, ^{209}Bi as a target



As the charge number of the projectile core increases, the Coulomb potential of the system increases (~Z1*Z2), reducing the probability of fusion.

Ca-Calcium (Z=20)	Fe-Iron (Z=26)	Ge-Germanium (Z=32)
Ti-Titanium (Z=22)	Ni-Nickel (Z=28)	Se-Selenium (Z=34)
Cr-Chromium (Z=24)	Zn-Zinc (Z=30)	Kr-Krypton (Z=36)

Nihonium (Image credit: AlexLMX | Shutterstock)

Japanese recognized for discovering element 113

Kosuke Morita points to element 113, which his team has earned the right to name.

January 1, 2016 01:46 JST

RIKEN-NC-NP-72

$^{70}Zn + ^{209}Bi \rightarrow ^{278}113 + n$

New Result in the Production and Decay of an Isotope, ^{278}113, of the 113th Element

Kosuke Morita[1*], Kouji Morimoto[1], Daiya Kaji[1], Hiromitsu Haba[1], Kazutaka Ozeki[1], Yuki Kudou[1], Takayuki Sumita[2,1], Yasuo Wakabayashi[1], Akira Yoneda[1], Kengo Tanaka[2,1], Sayaka Yamaki[3,1], Ryutaro Sakai[4,1], Takahiro Akiyama[3,1], Shin-ichi Goto[5], Hiroo Hasebe[1], Minghui Huang[1], Tianheng Huang[6], Eiji Ideguchi[7†], Yoshitaka Kasamatsu[1‡], Kenji Katori[1], Yoshiki Kariya[5], Hidetoshi Kikunaga[8], Hiroyuki Koura[9], Hisaaki Kudo[5], Akihiro Mashiko[10], Keita Mayama[10], Shin-ichi Mitsuoka[9], Toru Moriya[10], Masashi Murakami[5], Hirohumi Murayama[5], Saori Namai[10], Akira Ozawa[11], Nozomi Sato[9], Keisuke Sueki[11], Mirei Takeyama[10], Fuyuki Tokanai[10], Takayuki Yamaguchi[3], and Atsushi Yoshida[1]

Beamtime		Irradiation time (days)	Beam dose/sum ($\times 10^{19}$)	Number of observed events
year	month/day			
2003	9/5 12/29	57.9	1.24/1.24	0
2004	7/8 8/2	21.9	0.51/1.75	1
2005	1/20 1/23	3.0	0.07/1.82	0
2005	3/20 4/22	27.1	0.71/2.53	1
2005	5/19 5/21	2.0	0.05/2.58	0
2005	8/7 8/25	16.1	0.45/3.03	0
2005	9/7 10/20	39.0	1.17/4.20	0
2005	11/25 12/15	19.5	0.63/4.83	0
2006	3/14 5/15	54.2	1.37/6.20	0
2008	1/9 3/31	70.9	2.28/8.48	0
2010	9/7 10/18	30.9	0.52/9.00	0
2011	1/22 5/22	89.8	2.01/11.01	0
2011	12/2 12/19	14.4	0.33/11.34	0
2012	1/15 2/9	25.0	0.56/11.90	0
2012	3/13 4/17	33.7	0.79/12.69	0
2012	6/12 7/2	15.7	0.25/12.94	0
2012	7/14 8/18	32.0	0.57/13.51	1
Total		553	13.51	3

The experimental capability limit at that time (Japan):

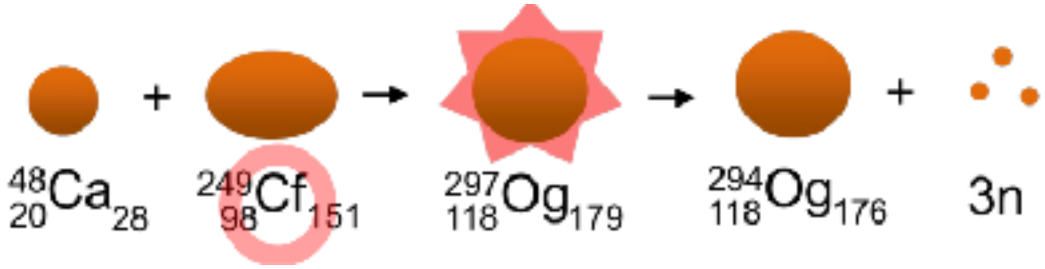
Beam intensity: ~$1 \mathrm{p}\mu\mathrm{A}$; $\sigma \sim 19\mathrm{fb}$

Result: 575 days, 3 events

Zn-Zinc (Z=30) Bismuth-209 femtobarn

Plutonium-244 **Ge-Germanium (Z=32)**

Hot fusion



$$^{48}\text{Ca} + ^{244}\text{Pu} \rightarrow Z = 114, \quad Z_1 \times Z_2 = 1880$$

$$^{76}\text{Ge} + ^{208}\text{Pb} \rightarrow Z = 114, \quad Z_1 \times Z_2 = 2624$$

the **Coulomb barrier** is about **40% weaker**,

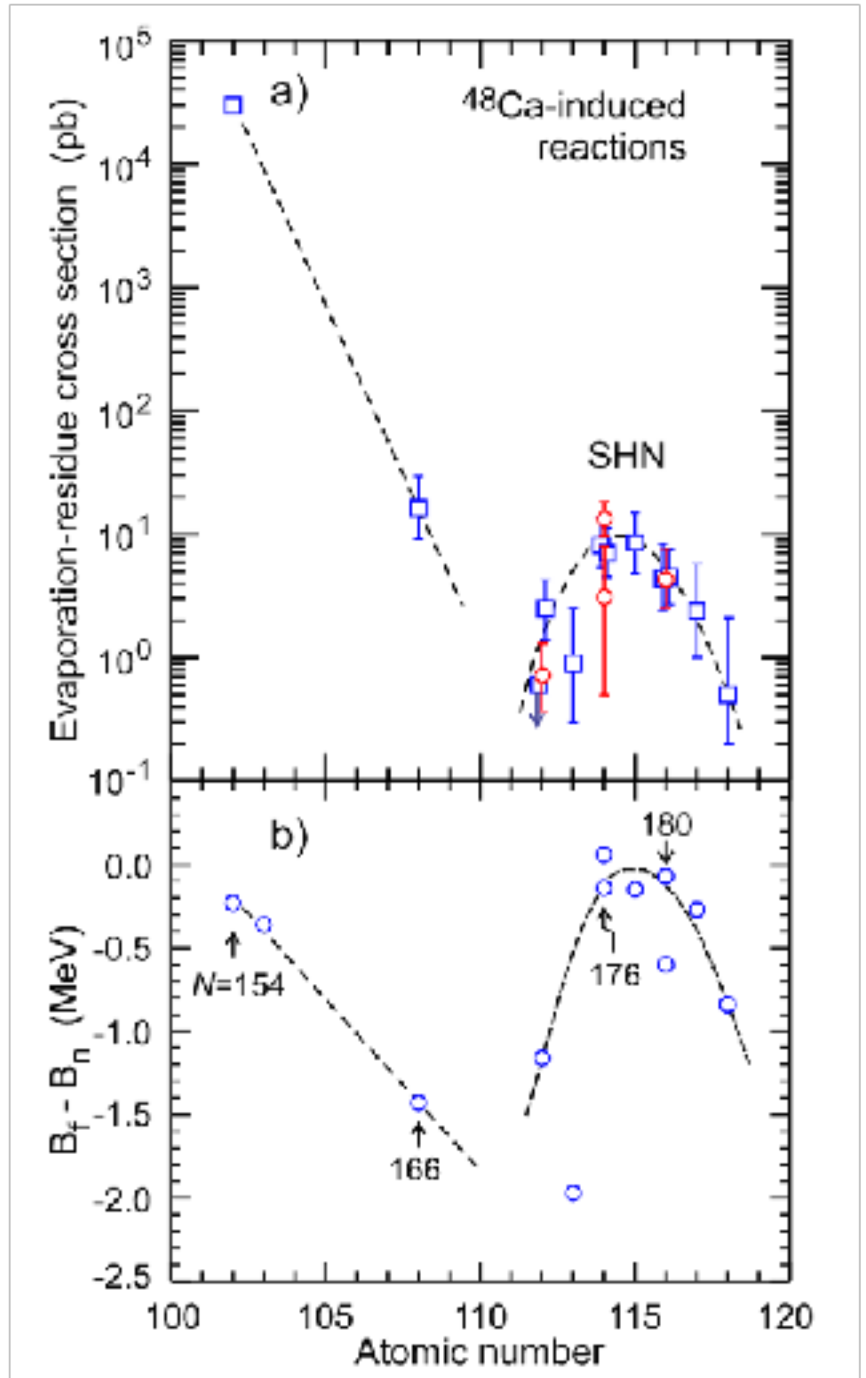
FLNR (Russia)

G.N. Flerov

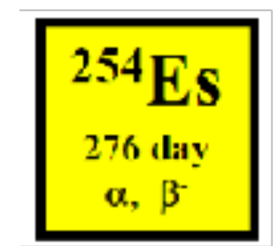
Yu.Ts. Oganessian

Fl (114)
Mc (115)
Lv (116)
Ts (117)
Og (118)
119,120
Synthesis
plan

Use ^{48}Ca as a beam



$$^{48}\text{Ca} + ^{254}\text{Es} \rightarrow Z = 119$$



唯一Z=99材料
仅有0.8微克

Es-Einsteinium (Z=99)

Yu.Ts. Oganessian, V.K. Utyonkov / Nuclear Physics A 944 (2015) 62–98

Content

- The history of Superheavy element production
- The challenge of Superheavy element production
- Bayesian uncertainty quantification for synthesizing superheavy element

元素	时间	实验室	反应体系
120	2009	Dubna	$^{58}Fe + ^{244}Pu$
120	2016	GSI	$^{54}Cr + ^{248}Cm$
119	2020	GSI	$^{50}Ti + ^{249}Bk$
120	2020	GSI	$^{50}Ti + ^{249}Cf$
119	2022	RIKEN	$^{51}V + ^{248}Cm$

Nothing has been observed yet

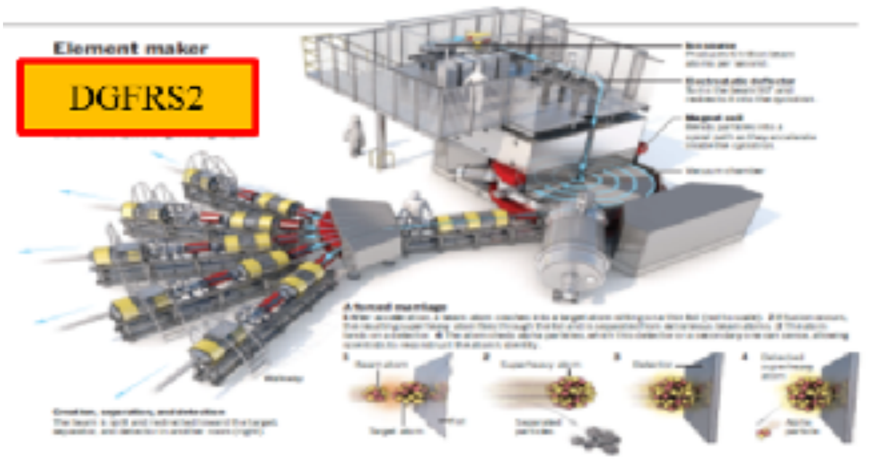
Beam intensity & Detection efficiency
Reaction system & Reaction energy

Experimental facilities for Z=119 and 120 elements in Russia, Japan, and China

Experimental challenges :

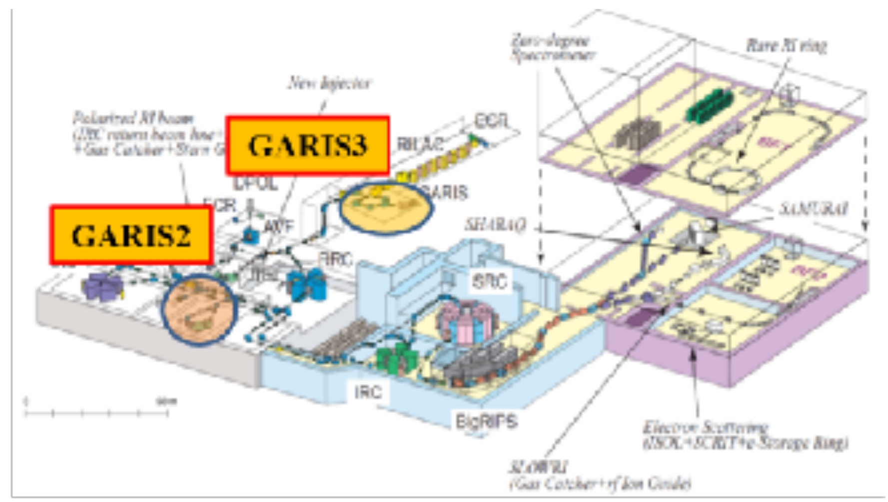
Higher beam intensity

Higher separation efficiency



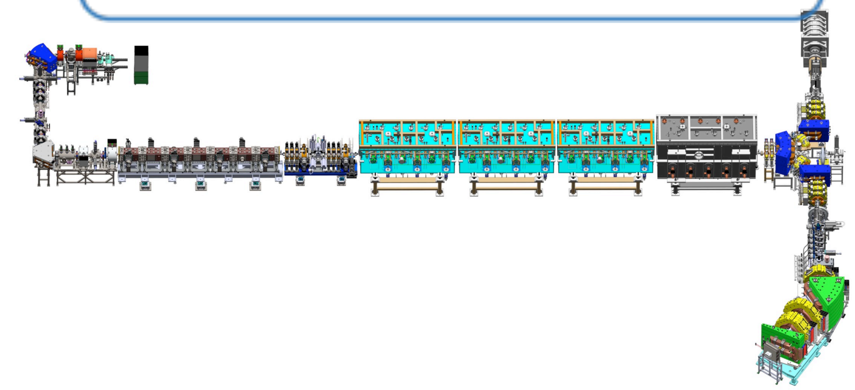
Russia JINR

SHE Factory + DGFRS2



Japan RIKEN

RILAC + GARIS3

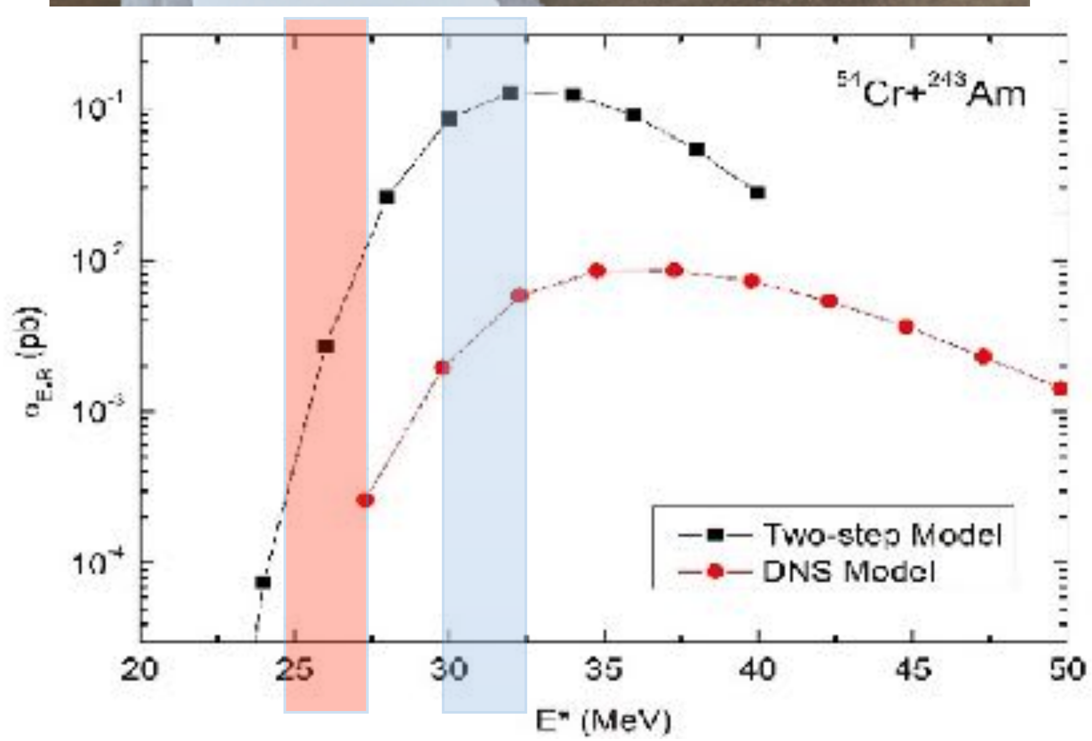


China IMP-CAS

CAFE2 + SHANS2

Country	Lab.	Facility	Beam intensity ($P\mu A$)	Efficiency
Russia	JINR	SHE Factory	~10	~59% ($^{48}Ca+^{206}Pb$)
Japan	RIKEN	RILAC	3~4	~47% ($^{40}Ar+^{169}Tm$)
China	**IMP-CAS**	**CAFE2**	**Now : 3~5** **Future : 10~15**	**~58% ($^{40}Ar+^{169}Tm$)**

The experimental capability limit at that time (Japan):
Beam intensity: ~$1p\mu A$; $\sigma \sim 19fb$



- **Research goal: Synthesize elements 119**

Try to synthesize element 119: 54Cr + 243Am

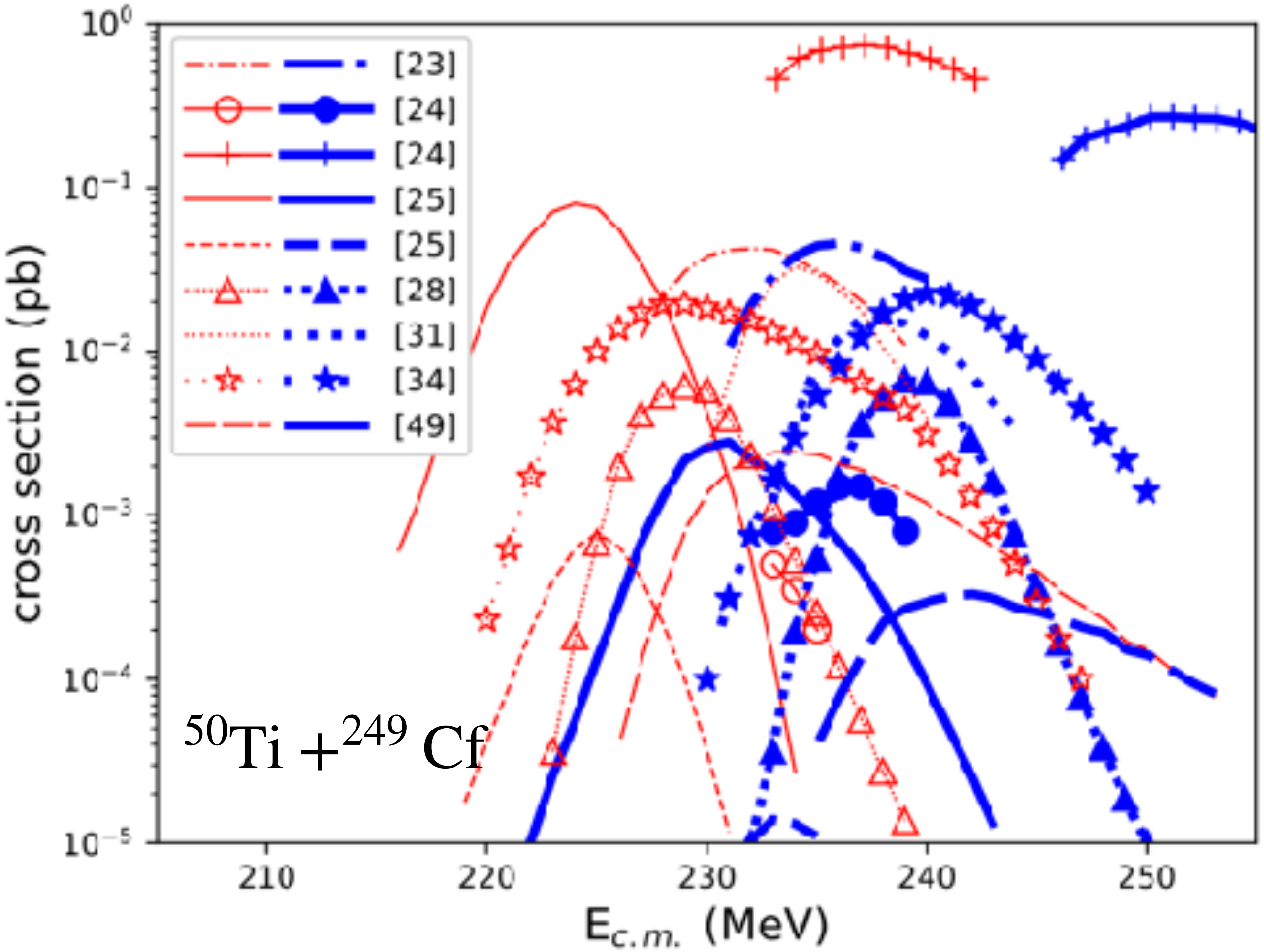
(Image credit: AlexLMX | Shutterstock)

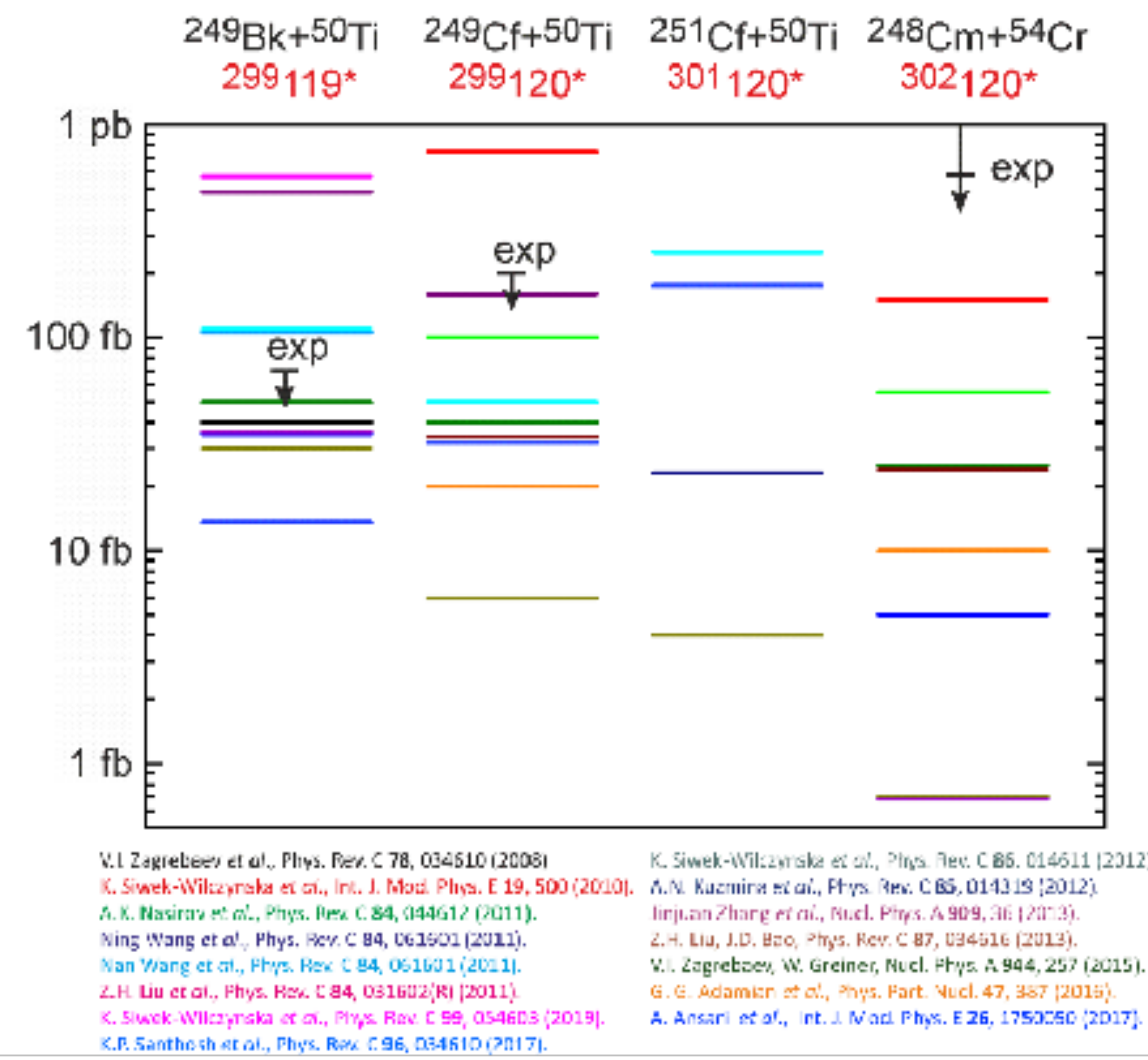
The experimental capability limit at that time (Japan):
Beam intensity: ~$1\mathrm{p}\mu\mathrm{A}$; $\sigma \sim 19$fb
Result: 575 days, 3 events

$\sigma \sim 8$fb, beam intensity $5 \sim 10\mathrm{p}\mu\mathrm{A}$
Standard experimental settings:
events/200~100 days, feasible!

From Zhang san's slide

Theoretical predictions for the production of element Z = 120 from the 3n (thin, red lines) and 4n (thick, blue lines) exit channels





Titanium-50

Californium-249

- **The cross-section error reaches 2-3 orders of magnitude**
- **10 MeV difference in optimum energy**

J. M. Gates, PhysRevLett.133.172502

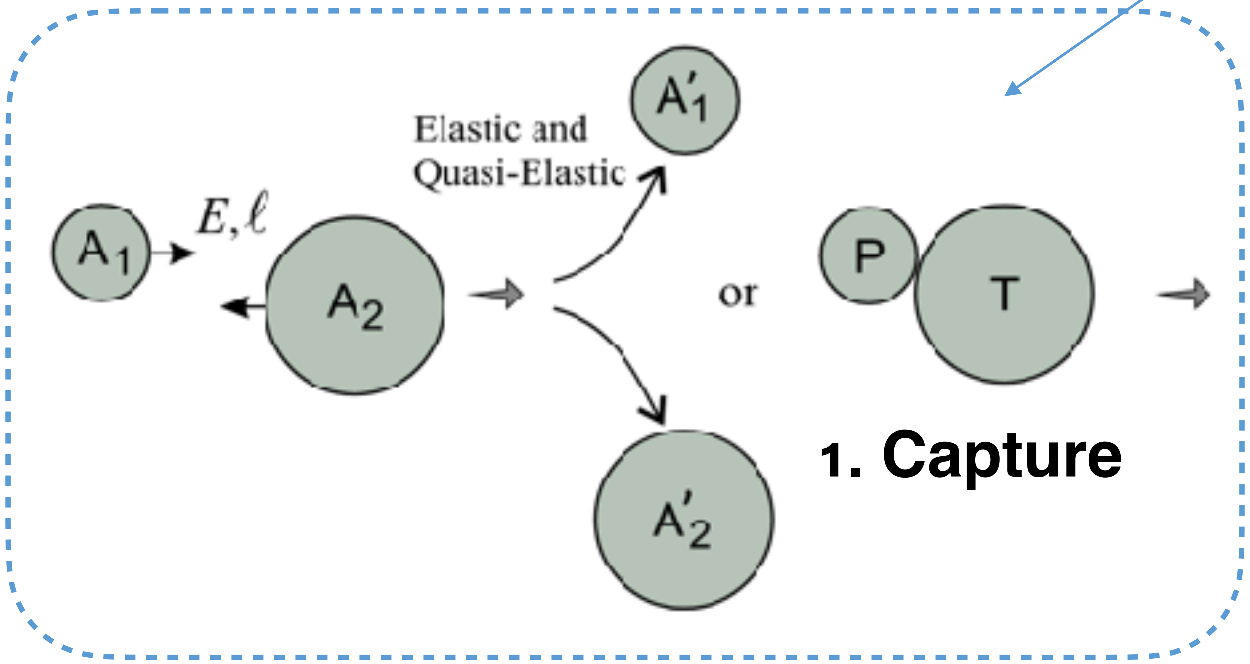
Content

- **The history of Superheavy element production**
- **The challenge of Superheavy element production**
- **Bayesian uncertainty quantification for synthesizing superheavy element** (Dinuclear **system model**)

Bayesian @ grid search

Aspect	Brute-force Sampling	Bayesian Inference
Concept	Uniformly or randomly samples	concentrate sampling in high-probability regions.
Efficiency	Highly inefficient in high dimensions	Highly efficient — focuses on the posterior distribution
Parameter Correlation	Ignores it entirely	Naturally captures and models parameter correlations via joint posterior distributions.
Uncertainty Quantification	Difficult — no built-in method for confidence intervals or credible regions.	Built-in — provides full probabilistic description, including credible intervals and joint correlations.

$$\sigma_{\mathrm{ER}}(E_{\mathrm{c.m.}}) = \frac{\pi\hbar^2}{2\mu E_{\mathrm{c.m.}}} \sum_J (2J+1) T(E_{\mathrm{c.m.}}, J) P_{\mathrm{CN}}(E_{\mathrm{c.m.}}, J) W_{\mathrm{sur}}(E_{\mathrm{c.m.}}, J)$$

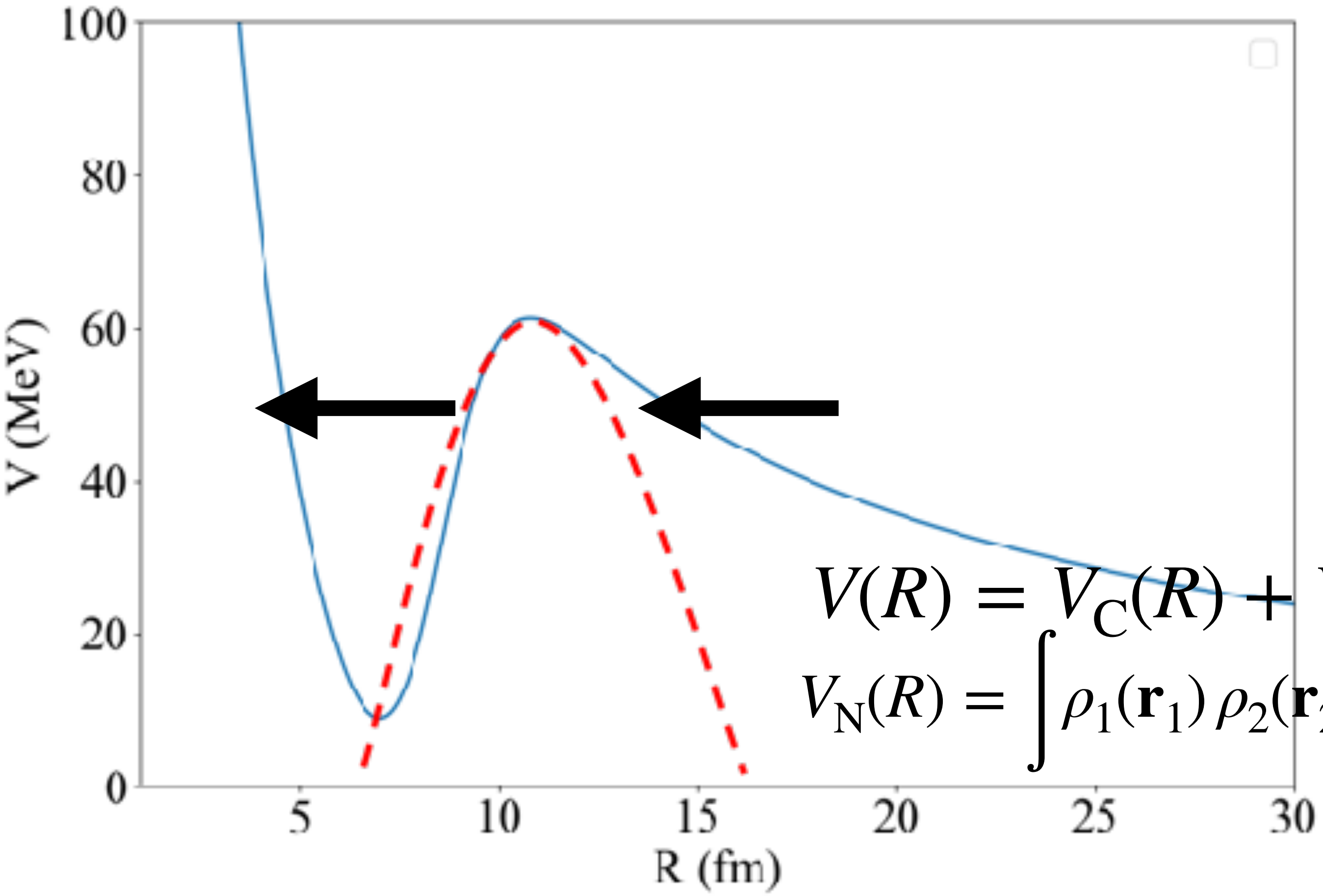


1. Capture

The transmission probability is calculated by using the Hill-Wheeler formula in combination with the barrier distribution function,

$$T_{\mathrm{cap}}(J, E_{\mathrm{c.m.}}) = \int \frac{f(B)dB}{1+\exp\{-\frac{2\pi}{\hbar\omega(J)}[E_{\mathrm{c.m.}} - B - \frac{\hbar^2}{2\mu R_B^2(J)} J(J+1)]\}},$$

$$f(B) = \begin{cases} \frac{1}{N}\exp\left[-\left(\frac{B-B_{\mathrm{m}}}{\Delta_1}\right)^2\right], & B < B_{\mathrm{m}}, \\ \frac{1}{N}\exp\left[-\left(\frac{B-B_{\mathrm{m}}}{\Delta_2}\right)^2\right], & B > B_{\mathrm{m}}. \end{cases}$$

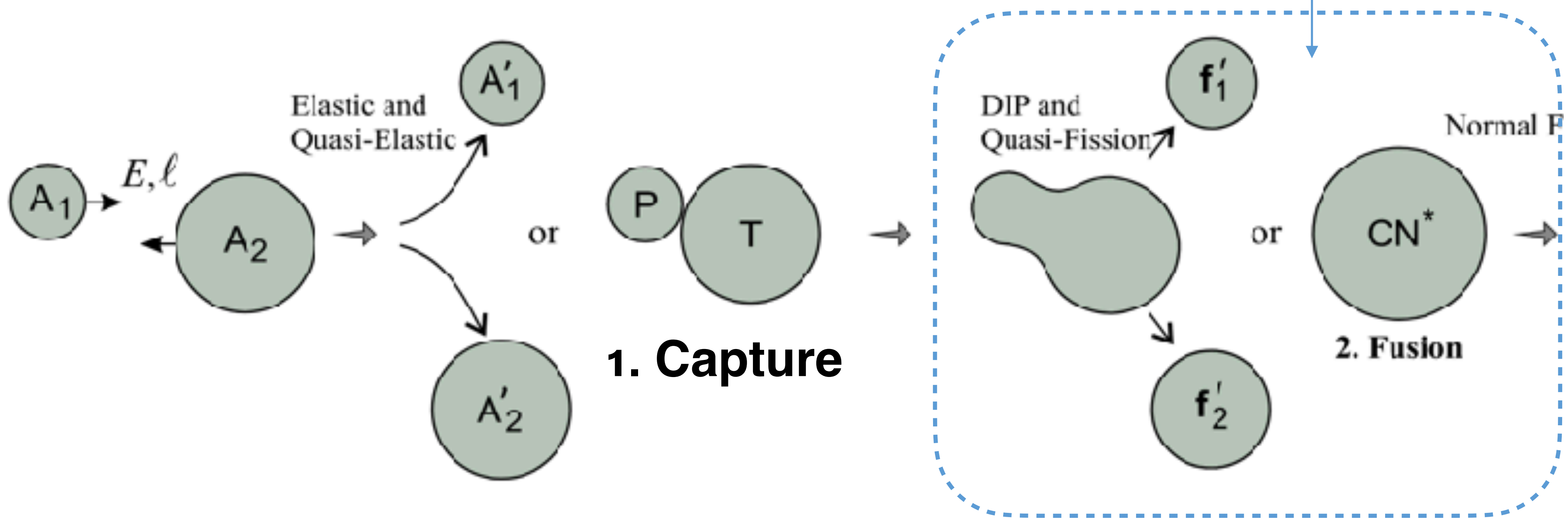


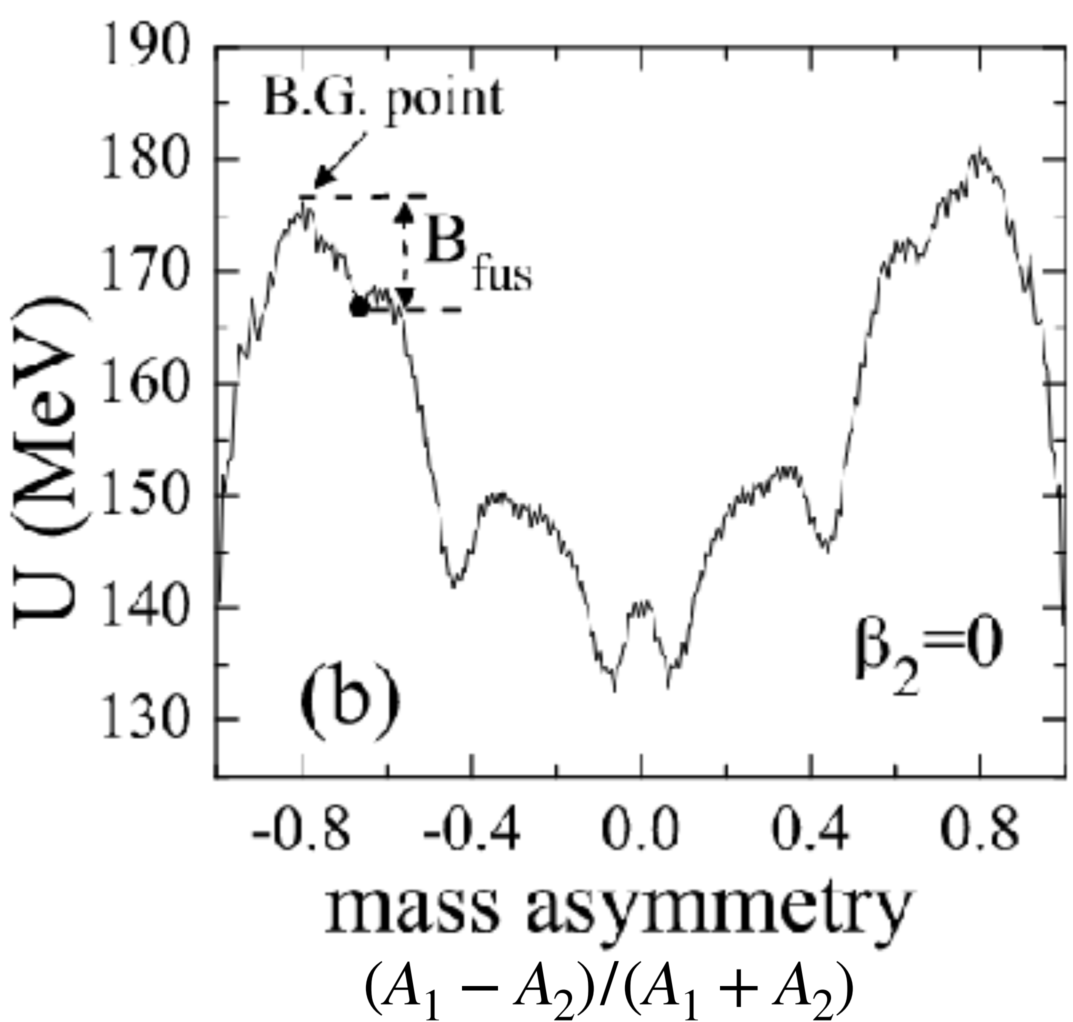
$$V(R) = V_{\mathrm{C}}(R) + V_{\mathrm{N}}(R)$$

$$V_{\mathrm{N}}(R) = \int \rho_1(\mathbf{r}_1)\,\rho_2(\mathbf{r}_2)\,v(\mathbf{r}_1 - \mathbf{r}_2 - \mathbf{R})\,\mathrm{d}\mathbf{r}_1\,\mathrm{d}\mathbf{r}_2$$

Bin Wang, Atomic Data and Nuclear Data Tables 114 (2017) 281‑370

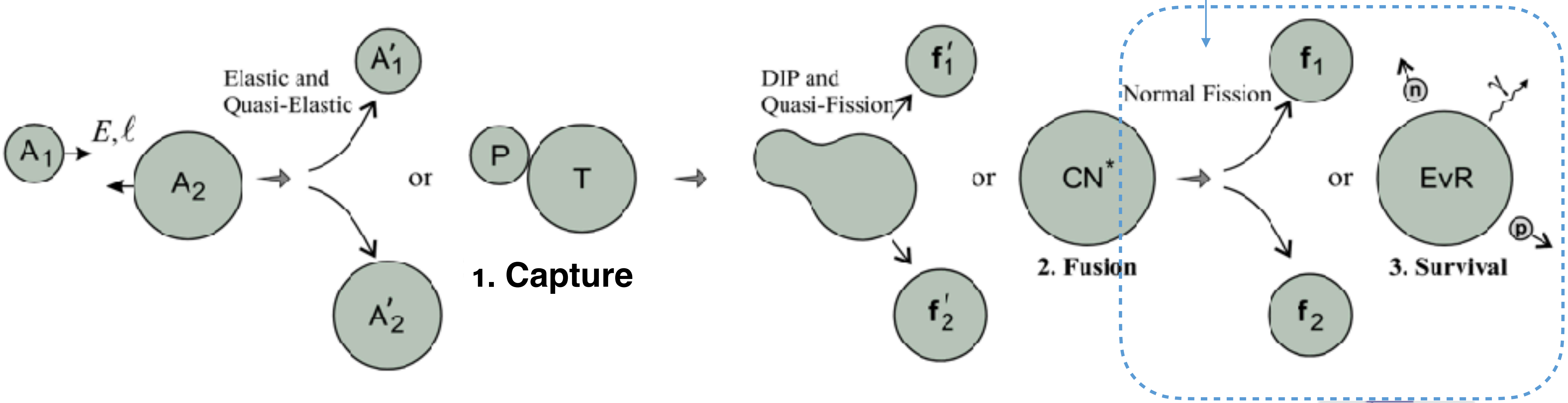
$$\sigma_{\mathrm{ER}}(E_{\mathrm{c.m.}}) = \frac{\pi\hbar^2}{2\mu E_{\mathrm{c.m.}}} \sum_J (2J+1) T(E_{\mathrm{c.m.}}, J) P_{\mathrm{CN}}(E_{\mathrm{c.m.}}, J) W_{\mathrm{sur}}(E_{\mathrm{c.m.}}, J)$$

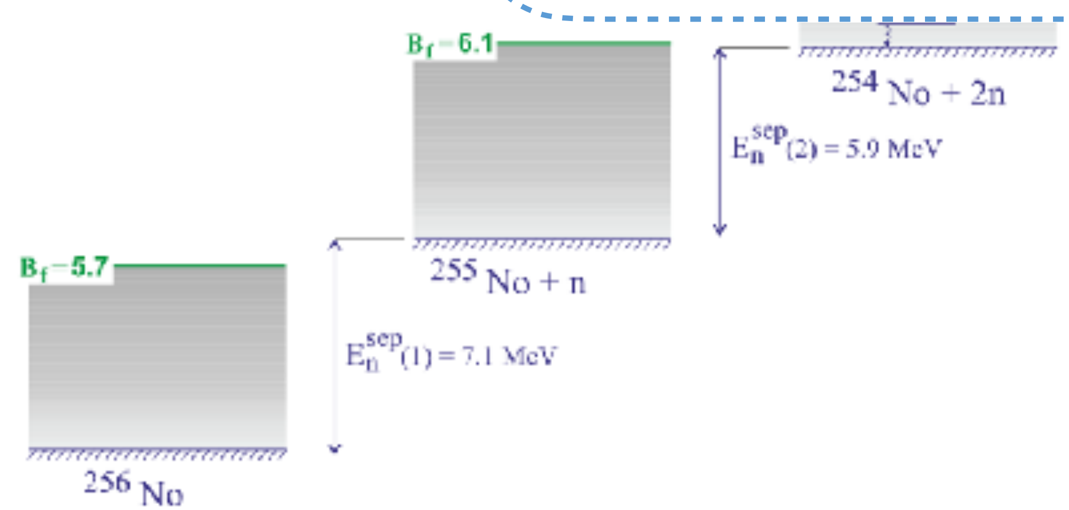




$$\begin{aligned}
&\frac{dP(Z_1, N_1, \beta_2, J, t)}{dt} \\
&= \sum_{Z_1'} W_{Z_1,N_1,\beta_2;Z_1',N_1,\beta_2}(t)\left[d_{Z_1,N_1,\beta_2} P(Z_1', N_1, \beta_2, J, t)\right. \\
&\quad \left. - d_{Z_1',N_1,\beta_2} P(Z_1, N_1, \beta_2, J, t)\right] \\
&\quad + \sum_{N_1'} W_{Z_1,N_1,\beta_2;Z_1,N_1',\beta_2}(t)\left[d_{Z_1,N_1,\beta_2} P(Z_1, N_1', \beta_2, J, t)\right. \\
&\quad \left. - d_{Z_1,N_1',\beta_2} P(Z_1, N_1, \beta_2, J, t)\right] \\
&\quad + \sum_{\beta_2'} W_{Z_1,N_1,\beta_2;Z_1,N_1,\beta_2'}(t)\left[d_{Z_1,N_1,\beta_2} P(Z_1, N_1, \beta_2', J, t)\right. \\
&\quad \left. - d_{Z_1,N_1,\beta_2'} P(Z_1, N_1, \beta_2, J, t)\right]. \qquad (3)
\end{aligned}$$

$$\sigma_{\mathrm{ER}}(E_{\mathrm{c.m.}}) = \frac{\pi\hbar^2}{2\mu E_{\mathrm{c.m.}}} \sum_J (2J+1) T(E_{\mathrm{c.m.}}, J) P_{\mathrm{CN}}(E_{\mathrm{c.m.}}, J) W_{\mathrm{sur}}(E_{\mathrm{c.m.}}, J)$$





$$P_s(E_i^*) = \frac{\Gamma_s(E_i^*)}{\Gamma_{\mathrm{tot}}(E_i^*)}, \Gamma_{\mathrm{tot}} = \Gamma_n + \Gamma_p + \Gamma_\alpha + \Gamma_\gamma + \Gamma_{\mathrm{f}}$$

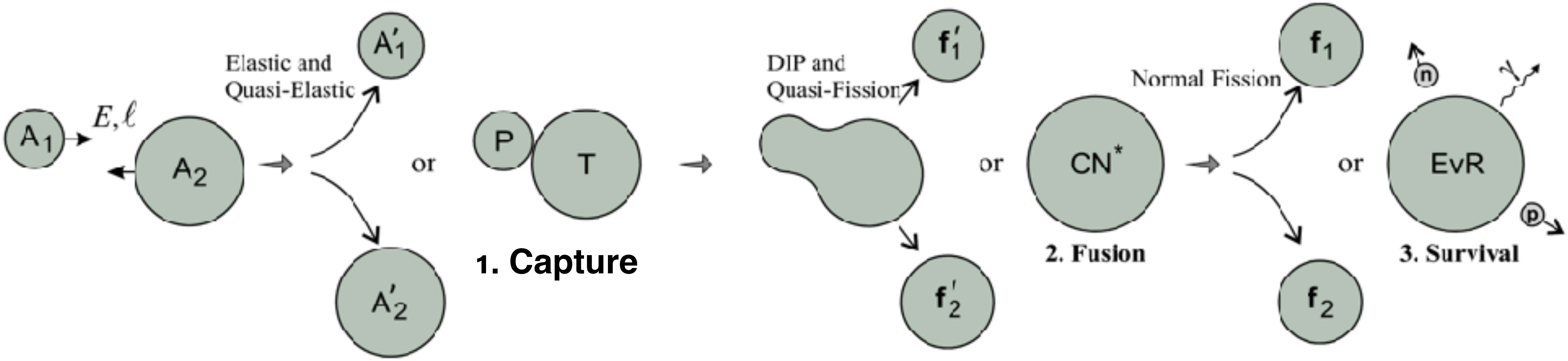
$$E_{i+1}^* = E_i^* - B_i$$

$$\Gamma_v(E^*, J) = \frac{(2s_v+1)m_v}{\pi^2\hbar^2\rho(E^*, J)} \times \int_0^{E^*-B_v} \epsilon\rho(E^* - B_v - \epsilon, J)\sigma_{inv}(\epsilon)d\epsilon \quad \sigma_{inv}(\epsilon) = \pi R^2$$

$$\Gamma_{\mathrm{f}}(E^*, J) = \frac{1}{2\pi\rho(E^*, J)} \times \int_0^{E^*-B_{\mathrm{f}}} \frac{\rho_{\mathrm{f}}(E^* - B_{\mathrm{f}} - \epsilon, J)}{1 + \exp[-2\pi(E^* - B_{\mathrm{f}} - \epsilon)/(\hbar\omega)]} d\epsilon$$

$$\rho(E^*, J) = K_{\mathrm{coll}} \frac{(2J+1)\sqrt{a}}{24(E^* - \delta - E_{\mathrm{rot}})^2} \left(\frac{\hbar^2}{\zeta}\right)^{3/2} \times \exp[2\sqrt{a(E^* - \delta - E_{\mathrm{rot}})}].$$

$$\sigma_{\mathrm{ER}}(E_{\mathrm{c.m.}}) = \frac{\pi\hbar^2}{2\mu E_{\mathrm{c.m.}}} \sum_J (2J+1) T(E_{\mathrm{c.m.}}, J) P_{\mathrm{CN}}(E_{\mathrm{c.m.}}, J) W_{\mathrm{sur}}(E_{\mathrm{c.m.}}, J)$$



Sensitivity Analysis and Parameter selection

参数	下限	上限
a (fm)	0.50	0.62
E_{d} (MeV)	12	32
$a_{\mathrm{f}}/a_{\mathrm{n}}$	0.95	1.20

$$\rho_1(\mathbf{r}, \theta_1) = \frac{\rho_0}{1 + \exp[(\mathbf{r} - \Re_1(\theta_1))/a_1]}$$

$$B_{\mathrm{f}}(E^*) = -E^0_{\mathrm{sh}} \mathrm{e}^{-E^*/E_{\mathrm{d}}}$$

$$\rho(E^*, J) = K_{\mathrm{coll}} \frac{(2J+1)\sqrt{a}}{24(E^* - \delta - E_{\mathrm{rot}})^2} \left(\frac{\hbar^2}{\zeta}\right)^{3/2} \times \exp[2\sqrt{a(E^* - \delta - E_{\mathrm{rot}})}] .$$

$$\alpha_{\mathrm{n}} = A/12\mathrm{MeV}^{-1}, \alpha_{\mathrm{f}}/\alpha_{\mathrm{n}}$$

We take 11, 10, and 7 points in their ranges, respectively, giving a total of 770 parameter sets. Based on the above parameter sets, we theoretically calculate the ERCS of the reactions $^{48}\mathrm{Ca} + ^{243}\mathrm{Am}$, for each set of parameters using the DNS model.

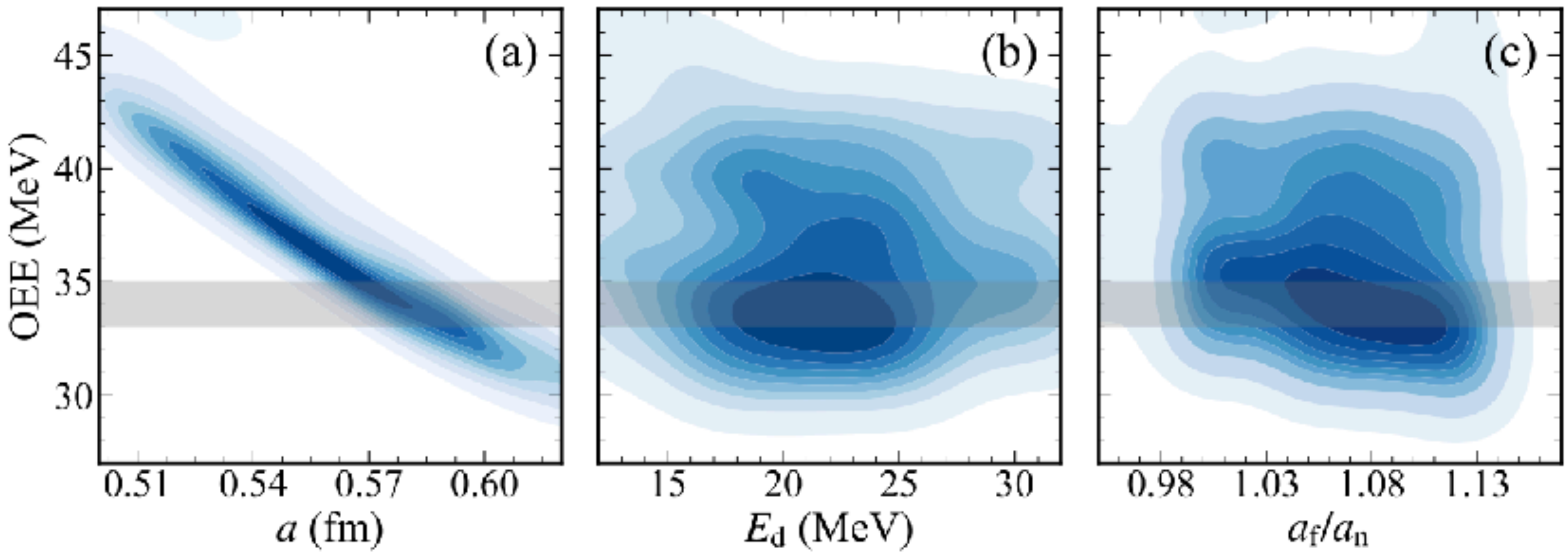
参数	下限	上限
a (fm)	0.50	0.62
E_d (MeV)	12	32
a_f/a_n	0.95	1.20

OEE = OIE + Q-value

OEE: optimal excition energy

OIE: optimal incident energy

Q value: use Myers mass table



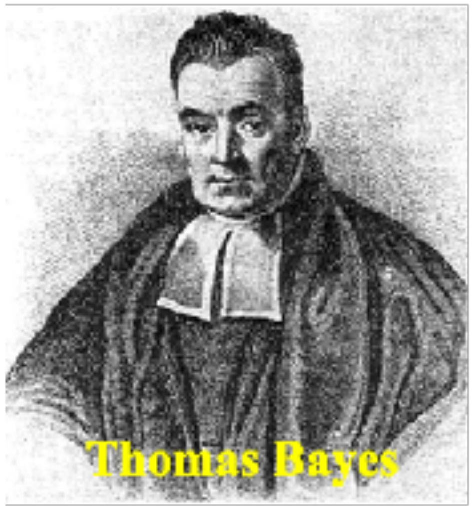
Gaussian process emulator

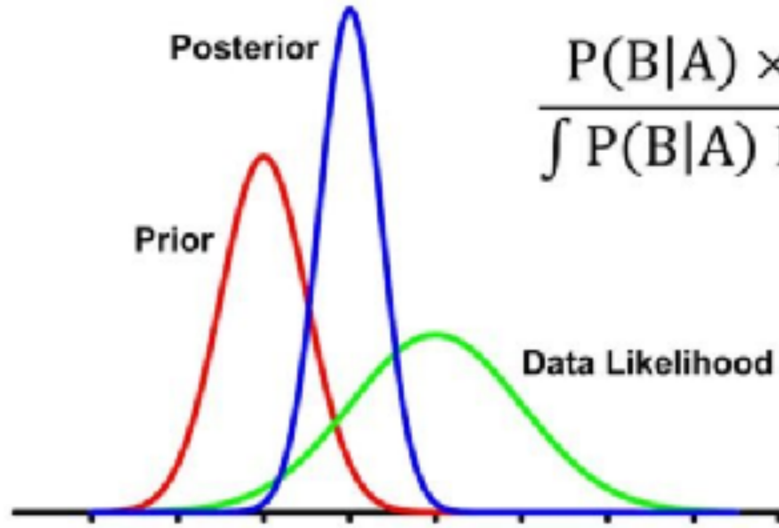
$$f(x) \sim \mathcal{GP}(m(x), k(x, x'))$$

- $m(x)$: mean function (often assumed to be zero)
- $k(x, x')$: covariance function or **kernel**, which defines how two input points are correlated

To output enough parameter sets

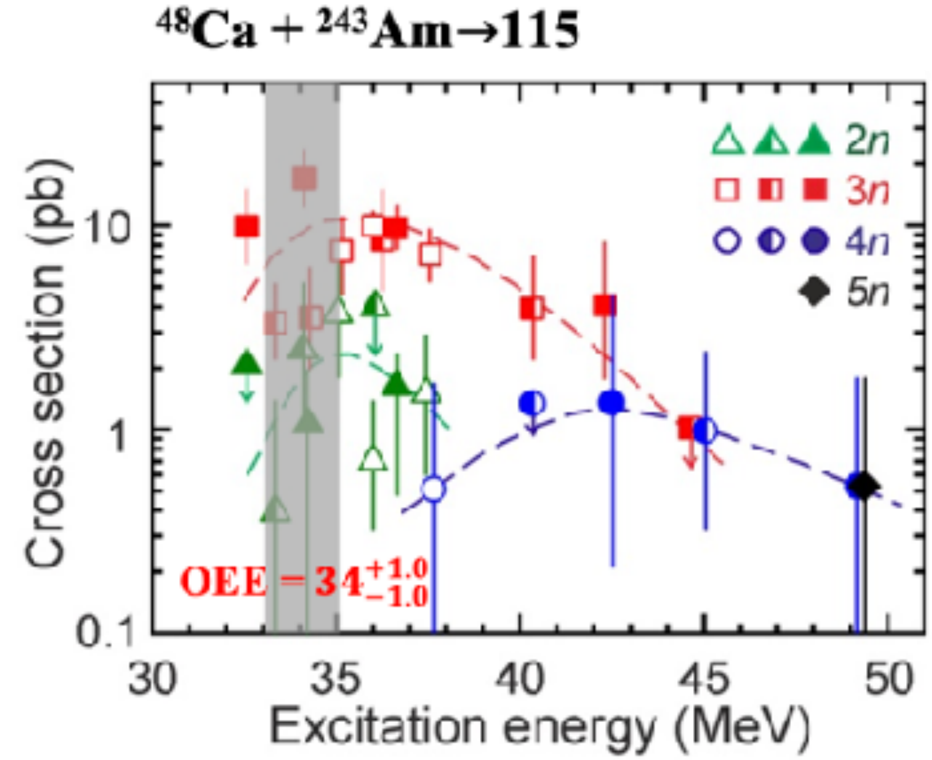
P. Möller, J. Nix, W. Myers, W. Swiatecki,, arXiv preprint arXiv:nucl-th/9308022, 1993.





$$\frac{P(B|A) \times P(A)}{\int P(B|A)\, P(A) dA}$$

Phys. Rev. C 99 (5) (2019) 054306.



$$P(\theta\,|\,\text{data}) \propto P(\text{data}\,|\,\theta) \cdot P(\theta)$$

$\theta = (a, E_d, a_f/a_n)$, **is the vector of model parameters to be inferred**

$P(\theta)$, **is the prior distribution of the parameters**

$P(\text{data}\,|\,\theta)$, **is the likelihood function, which quantifies how well the model predictions**

$$P(\text{Data}\,|\,X) \propto \exp\{-\frac{1}{2}(\text{Data}^{\text{emulator}} - \text{Data}^{\text{exp}})^{\text{T}} \sum_{\text{M}} (\text{Data}^{\text{emulator}} - \text{Data}^{\text{exp}})^{-1}\}$$

$P(\theta\,|\,\text{data})$, **is the posterior distribution**

Bayesian analysis provides a probabilistic framework for parameter estimation and uncertainty quantification, where all unknowns are treated as probability distributions.

MCMC method

In statistics, Markov chain Monte Carlo (MCMC) is a class of algorithms used to draw samples from a probability distribution.

Step-by-step:

1. Choose a starting point θ_0
2. For each step:
   - Propose a new point $\theta' \sim q(\theta' \mid \theta_t)$
   - Compute acceptance probability:

   $$\alpha = \min\left(1, \frac{P(\mathcal{D} \mid \theta')P(\theta')}{P(\mathcal{D} \mid \theta_t)P(\theta_t)} \cdot \frac{q(\theta_t \mid \theta')}{q(\theta' \mid \theta_t)}\right)$$

   - Accept or reject θ' with probability α
3. Store θ_{t+1}, repeat

This gives you a chain of samples that approximate the posterior $P(\theta \mid \mathcal{D})$

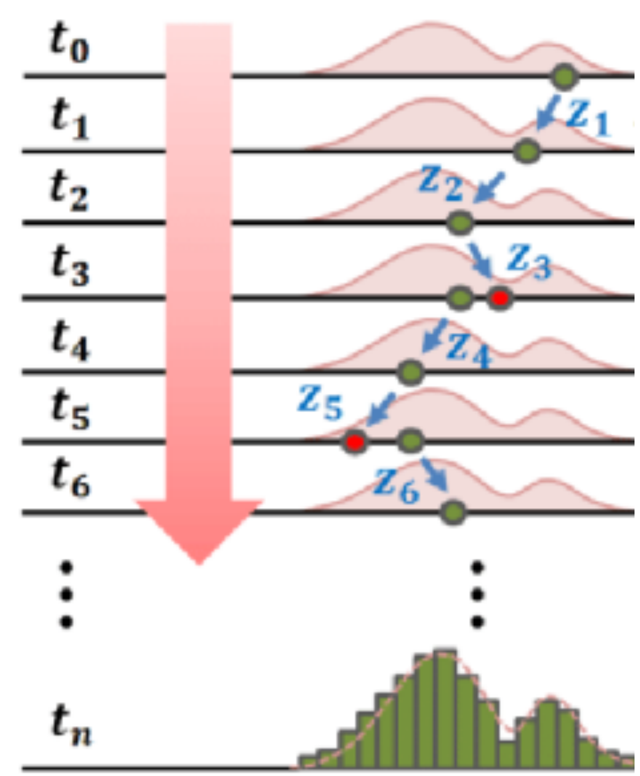
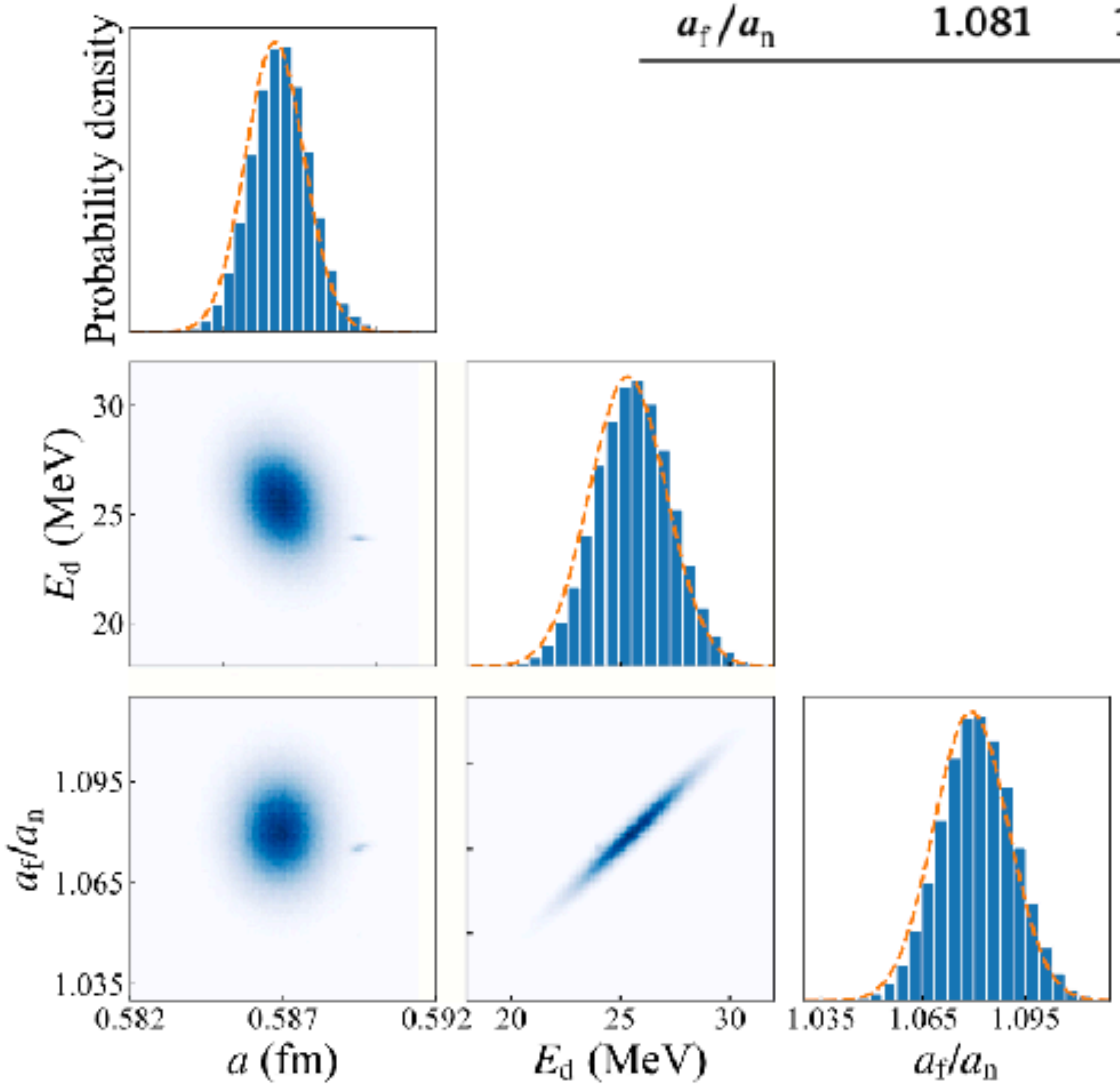


Illustration of Markov Chain Monte Carlo method

we build a full picture of the uncertainty and how parameters interact

The final state information of Bayesian inference
the posterior distribution of a, E_d, $a\_\mathrm{f}/a\_\mathrm{n}$

	mean	1σ	2σ
a (fm)	0.586	$0.586 \sim 0.587$	$0.585 \sim 0.589$
E_d (MeV)	25.65	$23.93 \sim 27.38$	$22.24 \sim 29.08$
$a_\mathrm{f}/a_\mathrm{n}$	1.081	$1.070 \sim 1.092$	$1.059 \sim 1.102$

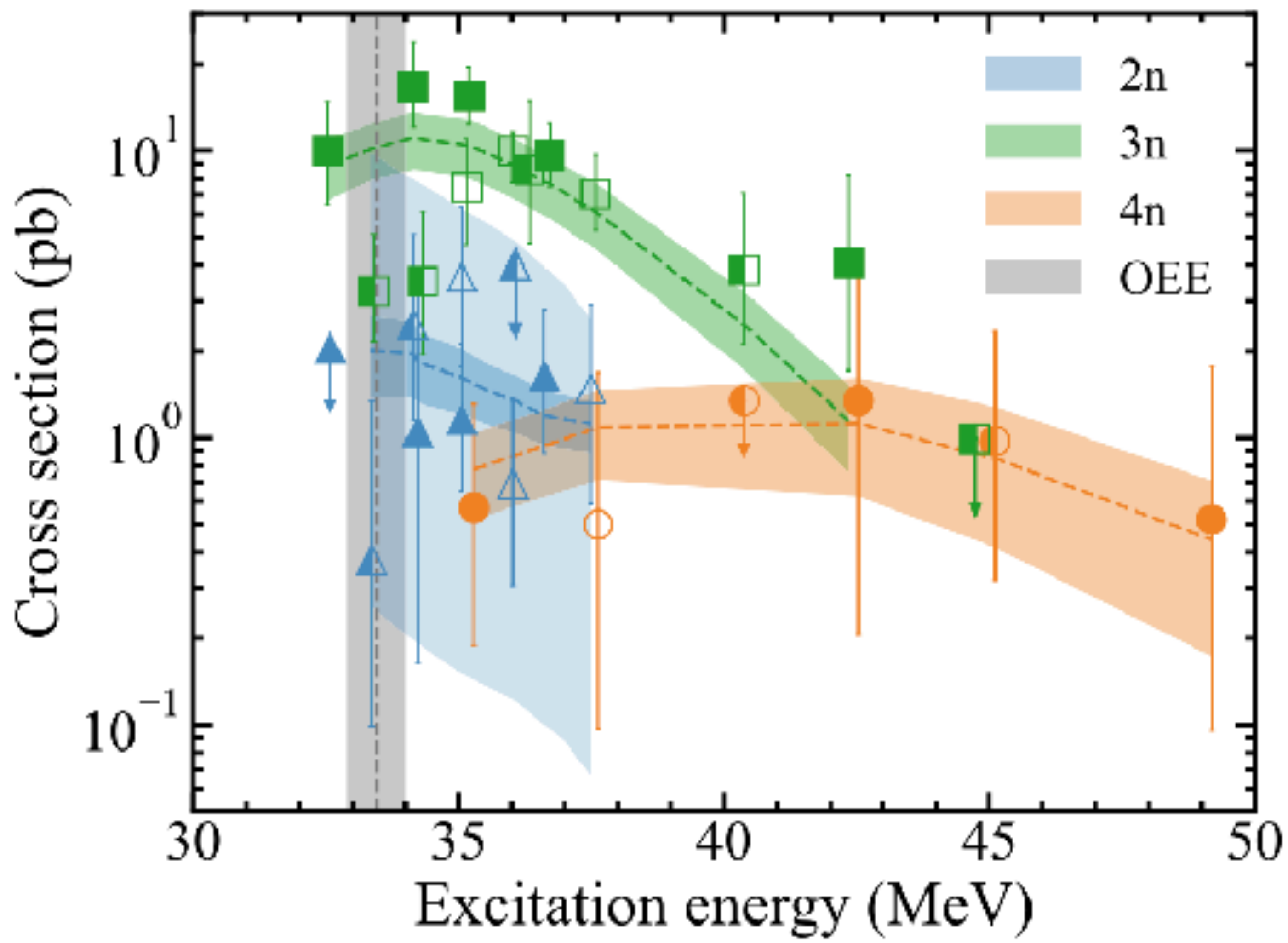


- There is a correlation between physical parameters. E_d is positively correlated with a_f/a_n, with a Pearson coefficient of 0.97.
- the key parameters is not independently

Final state information obtained by Bayesian inference

Calcium-48 plus Americium-243

$$^{48}\text{Ca} + ^{243}\text{Am} \rightarrow Z = 115$$



- **Under the 2σ confidence interval, the confidence intervals of ERCS for each n evaporation channel are within 1 order of magnitude**

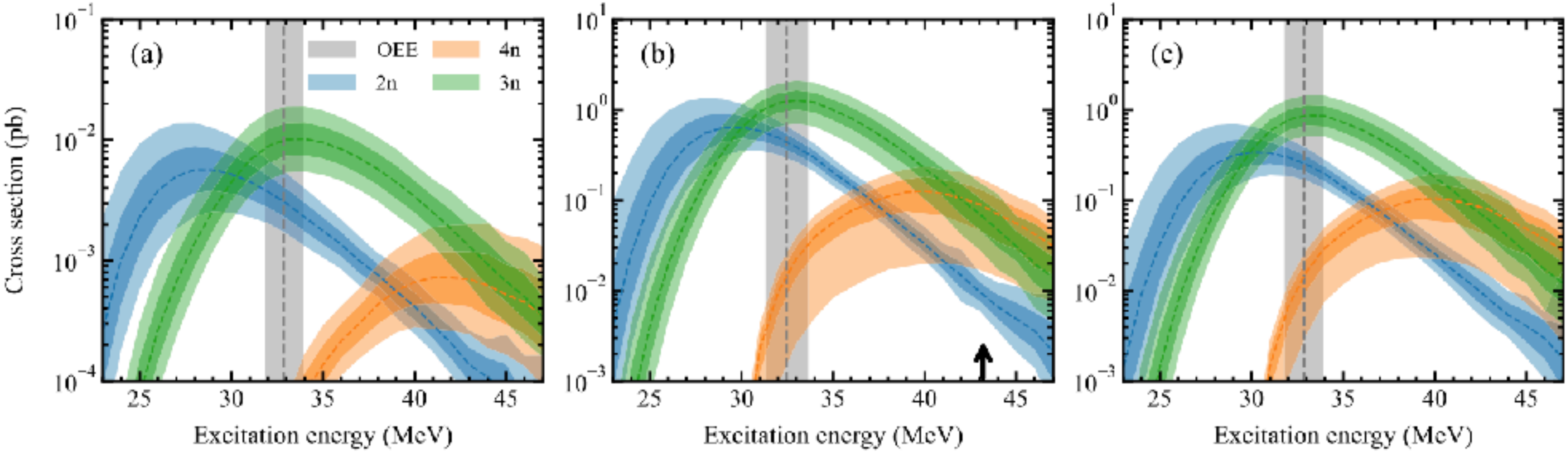
- **OIE confidence interval is $199.5 \sim 200.9$ MeV**

- **It is unreasonable to regard the correlation between parameters as independent**

OIE: optimal incident energy

Q = -165.99 MeV

$^{54}Cr + ^{243}Am \rightarrow Z = 119$ $^{50}Ti + ^{2449}Bk \rightarrow Z = 119$ $^{51}V + ^{248}Cm \rightarrow Z = 119$



Under the 2σ confidence interval, the confidence intervals of the ERCS of each n-evaporation channel are within 1 order of magnitude

- **(a)** $^{54}Cr + ^{243}Am \rightarrow Z = 119$ **OIE confidence interval is** $238.1 \sim 240.2$ **MeV**
- **(b)** $^{50}Ti + ^{2449}Bk \rightarrow Z = 119$ **OIE confidence interval is** $222.8 \sim 225.1$ **MeV**
- **(c)** $^{51}V + ^{248}Cm \rightarrow Z = 119$ **OIE confidence interval is** $227.1 \sim 229.3$ **MeV**

OEE = OIE + Q-value
OEE: optimal excition energy
OIE: optimal incident energy
Q value: use Myers mass table
Q **values for the reactions are -206.28, -191.47, and -195.34 MeV**

Summary

Discrepancies among theoretical models highlight the urgent need to quantify model uncertainties and improve theoretical reliability before guiding future experiments.

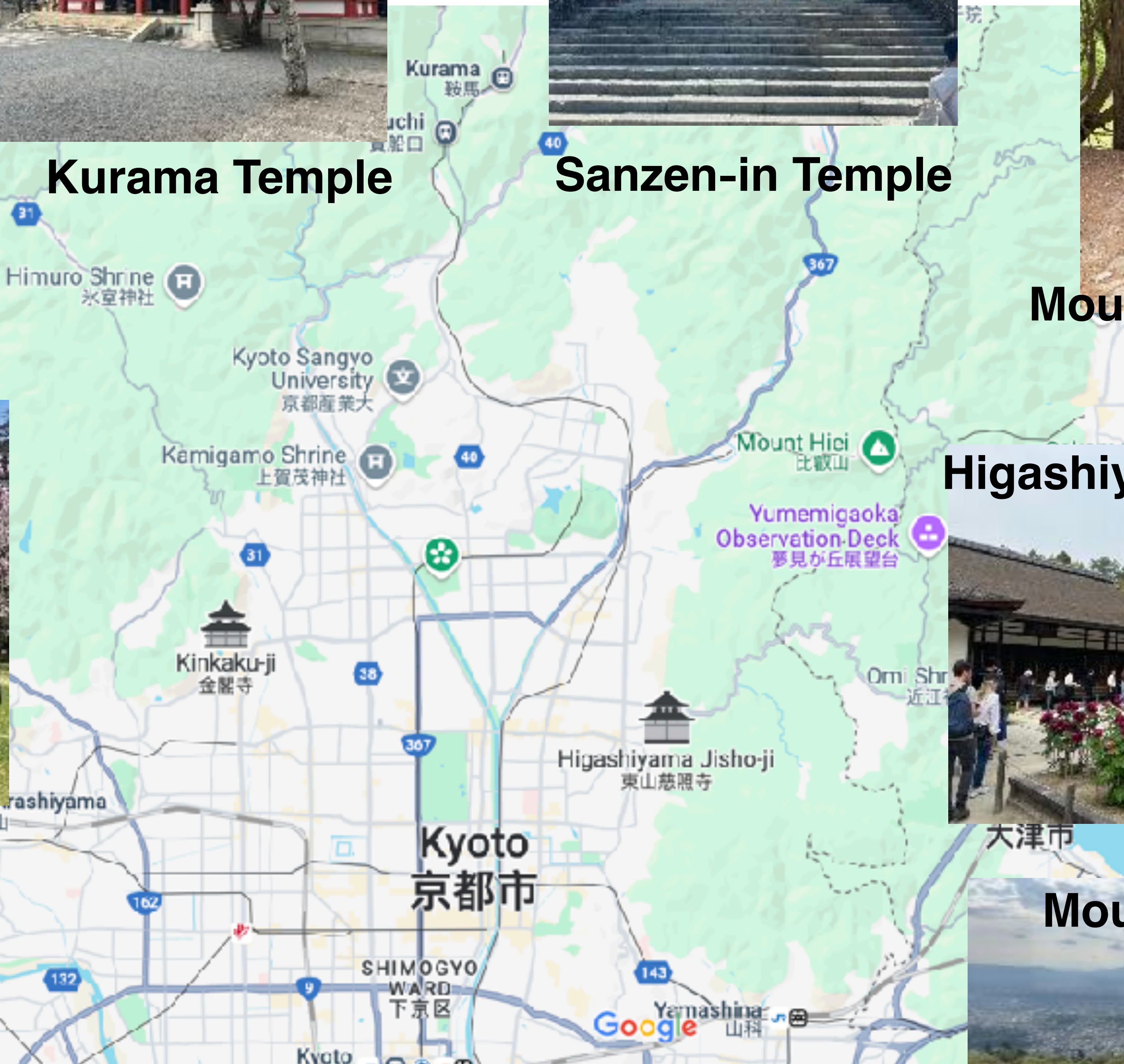
We have presented a comprehensive application of Bayesian inference method to the calculation and propagation of the key parameters' uncertainties in the DNS model.

	mean	1σ	2σ
a (fm)	0.586	$0.586 \sim 0.587$	$0.585 \sim 0.589$
E_{d} (MeV)	25.65	$23.93 \sim 27.38$	$22.24 \sim 29.08$
$a_{\mathrm{f}}/a_{\mathrm{n}}$	1.081	$1.070 \sim 1.092$	$1.059 \sim 1.102$

(a) $^{54}\mathrm{Cr} + ^{243}\mathrm{Am} \rightarrow Z = 119$ **OIE confidence interval is** $238.1 \sim 240.2$ **MeV**

(b) $^{50}\mathrm{Ti} + ^{2449}\mathrm{Bk} \rightarrow Z = 119$ **OIE confidence interval is** $222.8 \sim 225.1$ **MeV**

(c) $^{51}\mathrm{V} + ^{248}\mathrm{Cm} \rightarrow Z = 119$ **OIE confidence interval is** $227.1 \sim 229.3$ **MeV**



Arashiyama

Kurama Temple

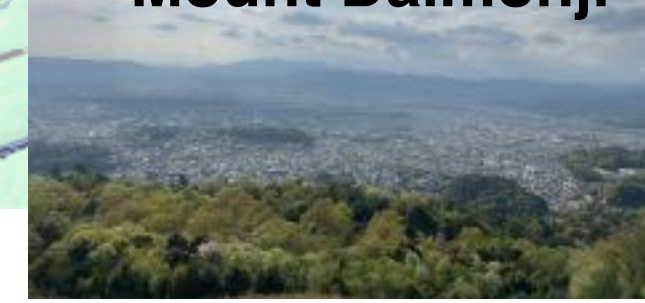
Sanzen-in Temple

Mountain Hiei

Kamigamo shrine

Higashiyama jisho-ji

Mount Daimonji



if you have some recommendation, please let me know !

If you also want to join me, please let me know !

arXiv:2107.01590v2

Gaussian process emulator

A **Gaussian Process (GP)** is a distribution over functions:

$$f(x) \sim \mathcal{GP}(m(x), k(x, x'))$$

- $m(x)$: mean function (often assumed to be zero)
- $k(x, x')$: covariance function or **kernel**, which defines how two input points are correlated

Given some training data $D = \{X, y\}$, and a new test point x_*, the GP posterior prediction is a norma distribution:

$$f(x_*) \sim \mathcal{N}(\mu(x_*), \sigma^2(x_*))$$

- $\mu(x_*)$: predictive mean
- $\sigma(x_*)$: predictive uncertainty