

原子核密度汎関数法に基づく 超重核の生成、核分裂の記述

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Superheavy element (SHE)

Relation between SHE and r-process

Fission of heavy, superheavy nuclei, ambiguity

Nuclear density functional theory (DFT)

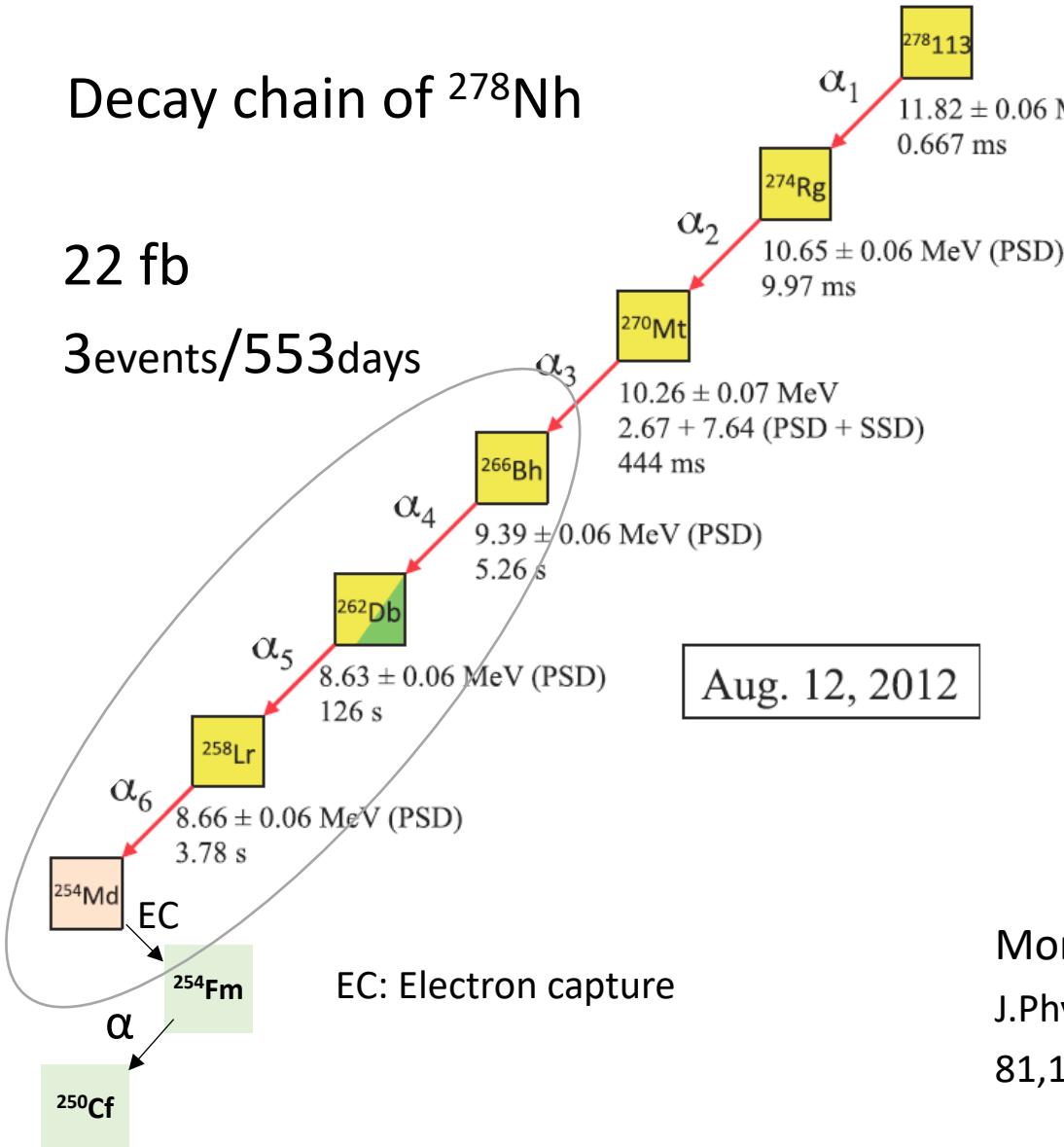
Study of fission and fusion

Introduction: Superheavy element (SHE)

Decay chain of ^{278}Nh

22 fb

3 events/553 days



Decay chain is connected to known nuclides ^{266}Bh , ^{262}Db , ^{258}Lr



Strong proof to synthesize ^{278}Nh

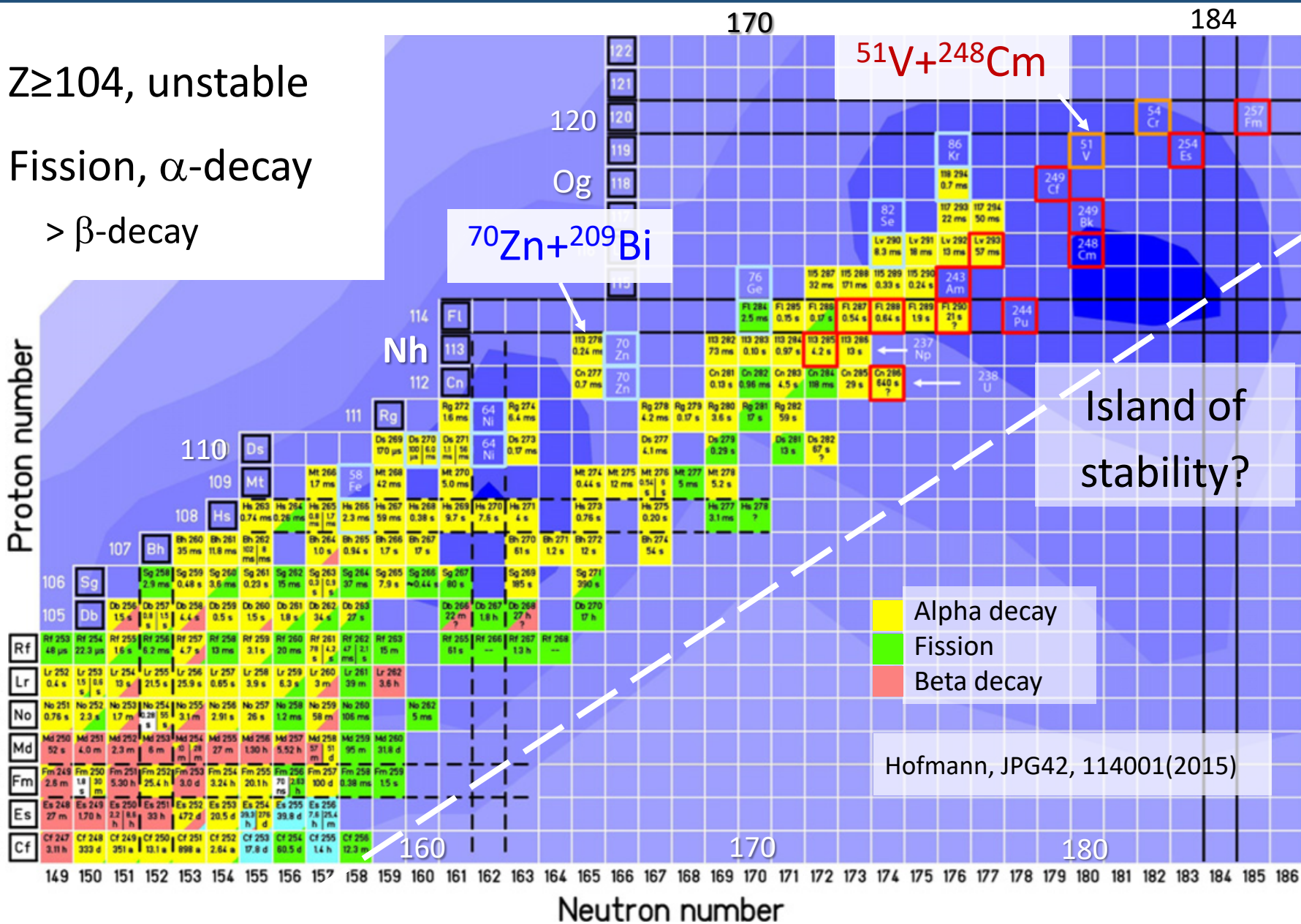
Morita et al.,
J.Phys.Soc.Jpn.
81,103201(2012)

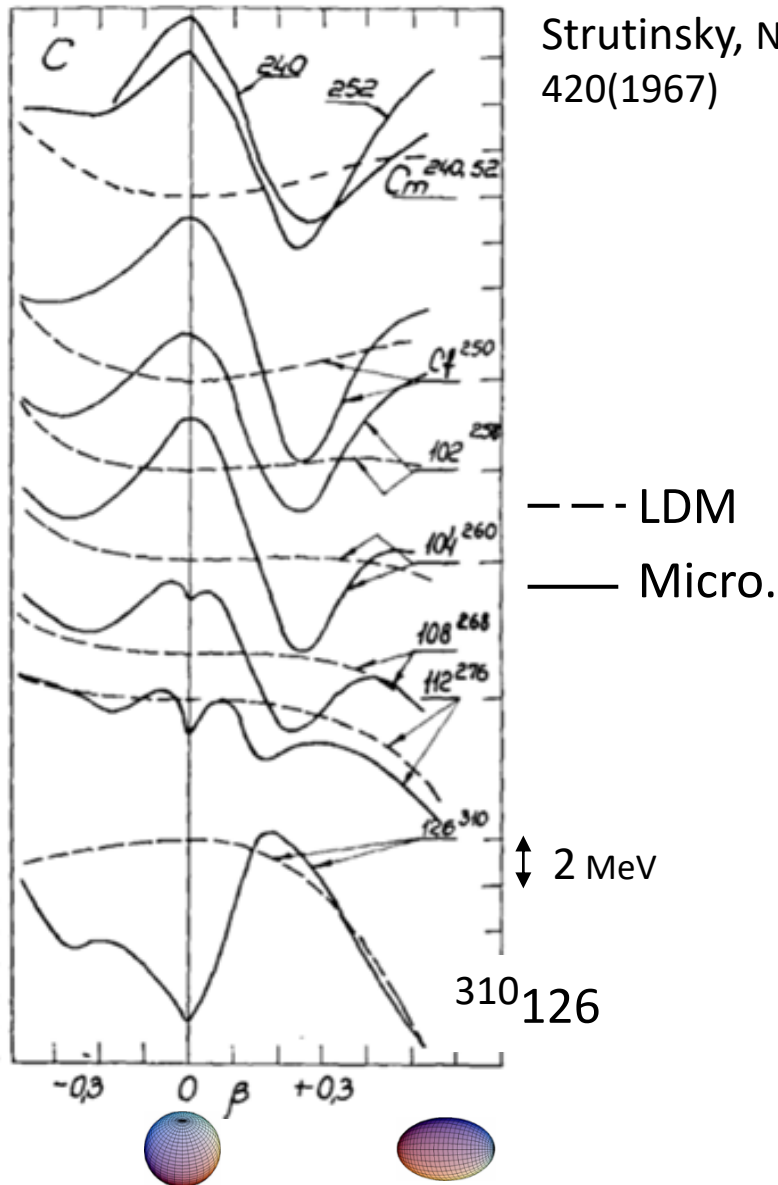
Basic properties of Superheavy elements

$Z \geq 104$, unstable

Fission, α -decay

$> \beta$ -decay



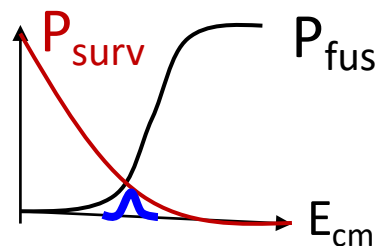


- Fission barrier by macroscopic liquid-drop model is lost in SHE
- Only microscopic models give a finite barrier -> Shell effect
- Next magic numbers

Z=114, 120, 126? N=184?

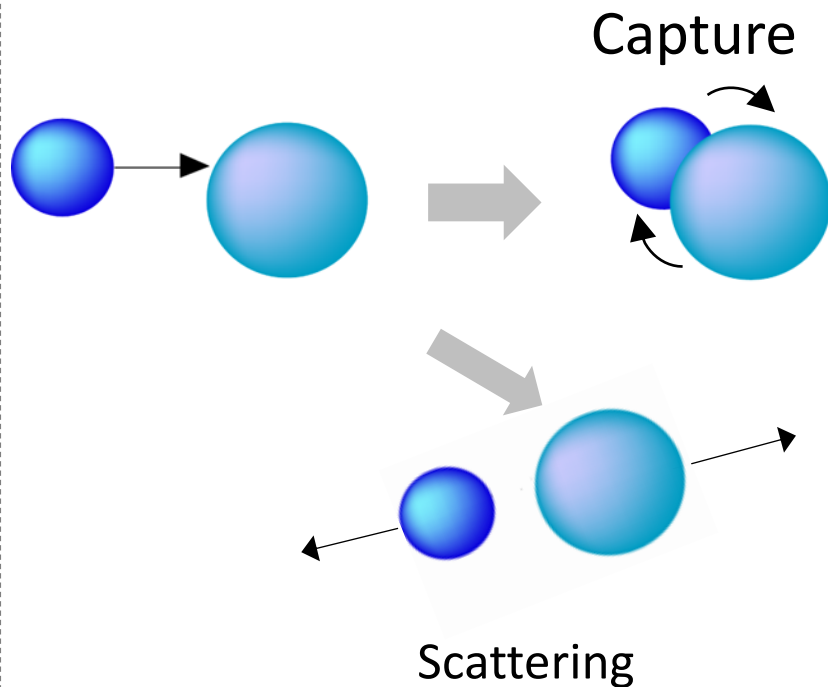
Formation of superheavy elements

$Z \leq 118$ have been synthesized by heavy-ion fusion reactions

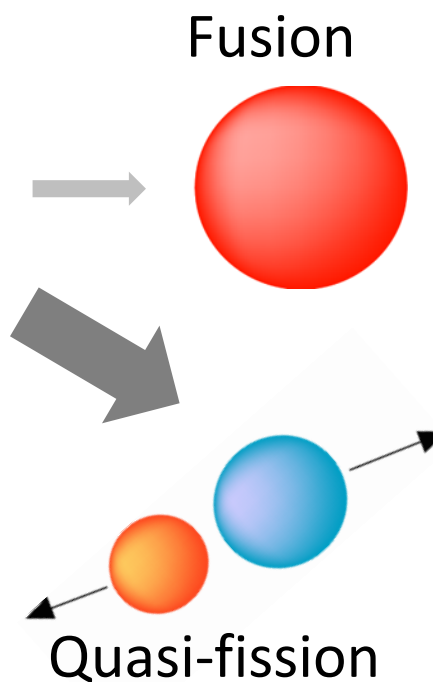


$$P_{ER} = P_{fus} \times P_{surv}$$

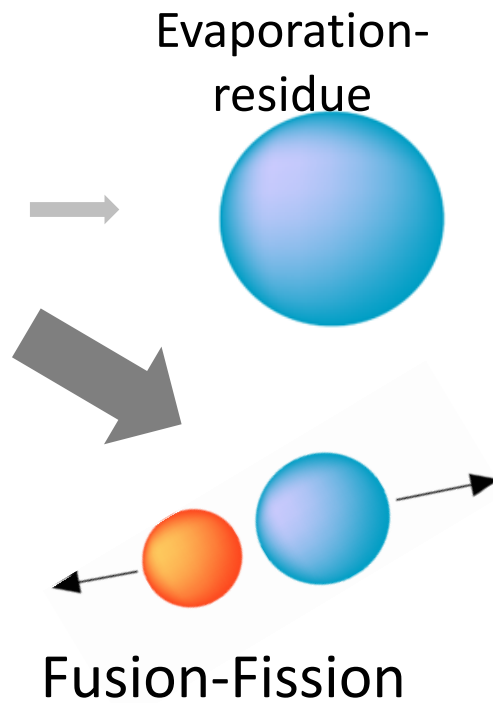
First stage



Second stage

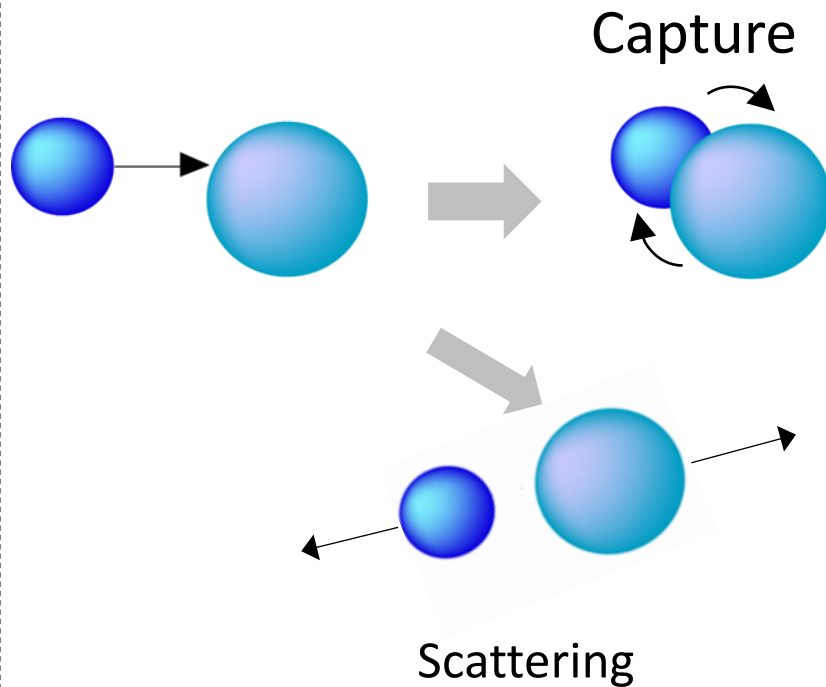


Third stage

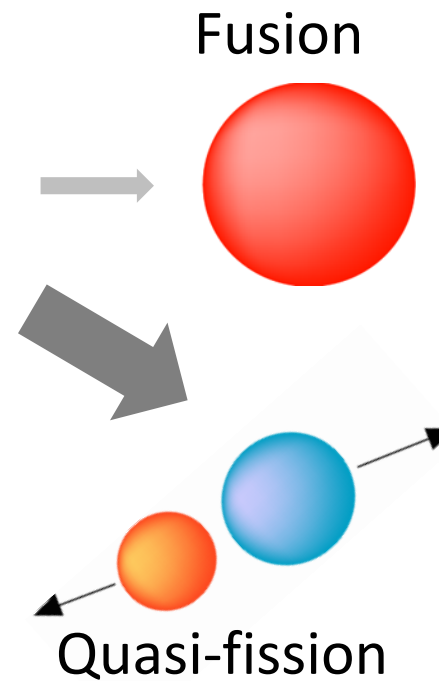


Fission is dominant process over SHE synthesis

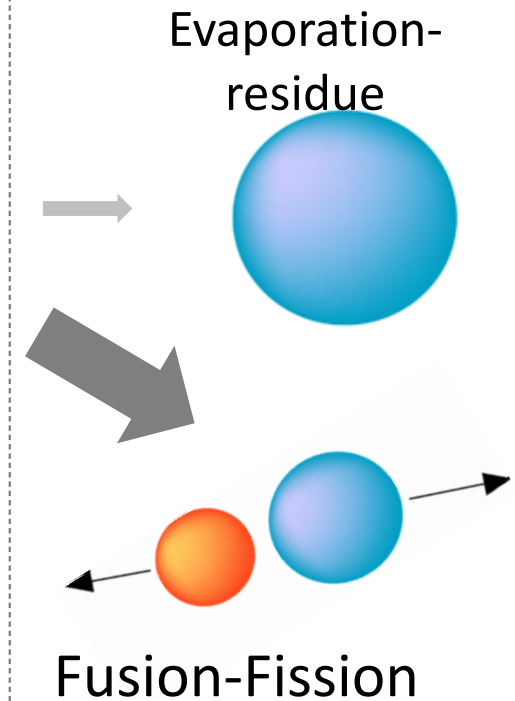
First stage



Second stage

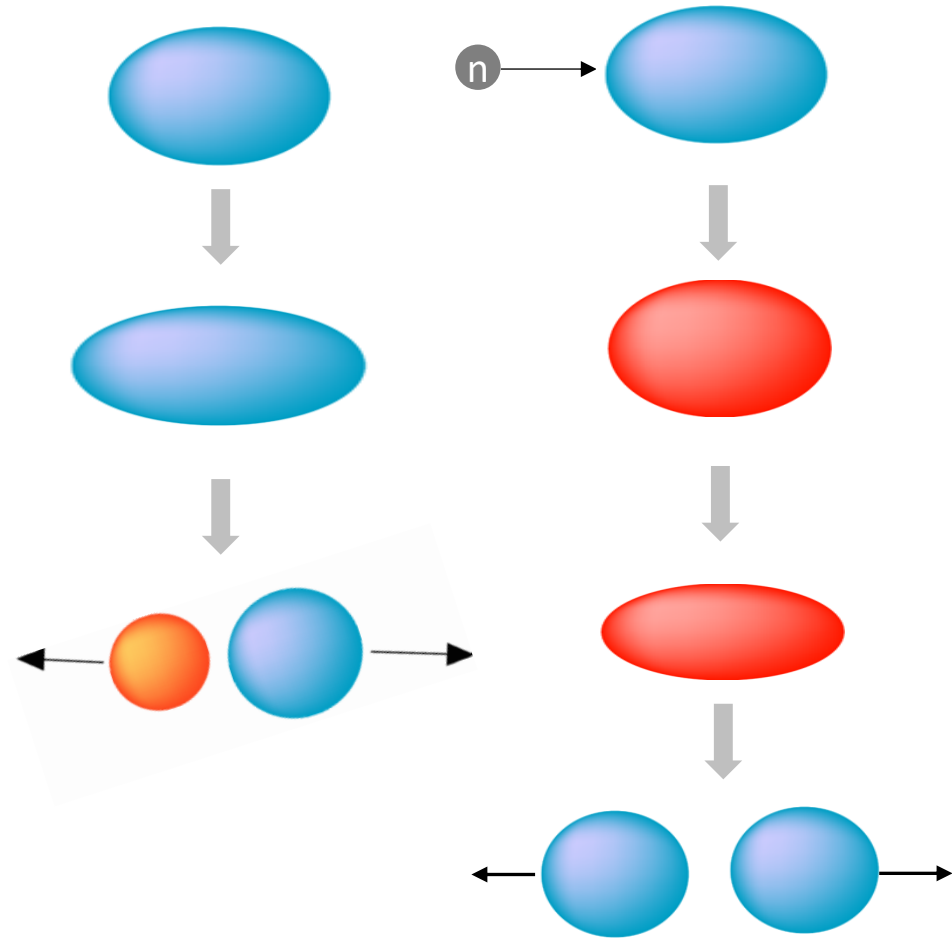
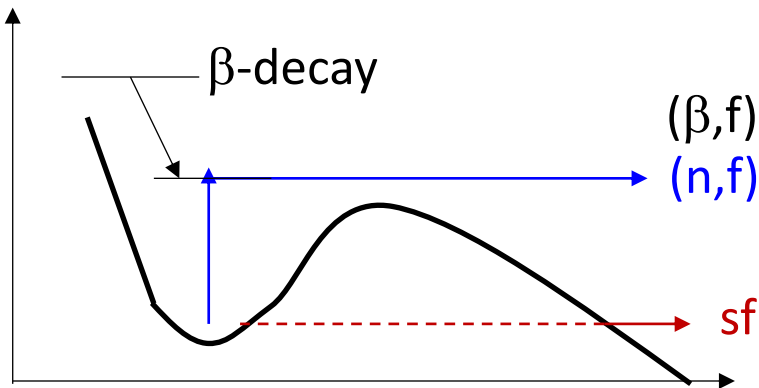


Third stage



Different types of fission relevant to r-process

- Spontaneous fission (**sf**)
- Neutron-induced fission (**n,f**)
- β -delayed fission (β ,f)
- Other



Hohenberg, Kohn, Phys. Rev. 136 (1964) B864 ~19000 citations
Kohn, Sham, Phys. Rev. 140 (1965) A1133 ~24000 citations

Many-body problem \rightarrow One-body potential
with non-interacting system

$E[\rho] \leftrightarrow \rho$ Energy is written by functional of density

$v(\mathbf{r}) \leftrightarrow |\Psi_0\rangle \leftrightarrow \rho_0(\mathbf{r})$ One to one correspondence between one-body potential, ground state, and density

$E_0 = \min_{\rho} E[\rho]$ The ground state energy is obtained by variational principle

Nuclear density functional exists, but its shape is unknown

Skyrme, Gogny, Covariant, etc.

Bender, Heenen, Reinhard, Rev. Mod. Phys. 75 (2003) 121
Nakatsukasa, Matsuyanagi, Matsuo, Yabana, RMP88(2016) 045004

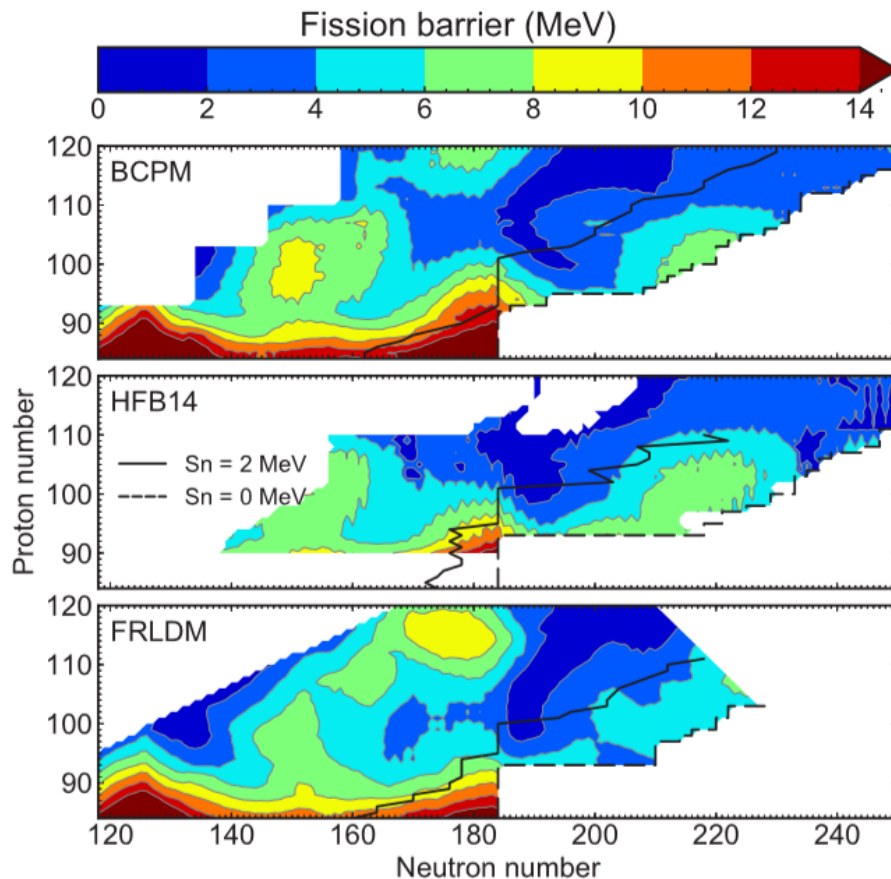
Fission properties of superheavy nuclei for r -process calculations

Phys.Rev.C97,034323 (2018)

 Samuel A. Giuliani,^{1,*} Gabriel Martínez-Pinedo,^{1,2,†} and Luis M. Robledo^{3,‡}
¹Institut für Kernphysik (Theoriezentrum), Technische Universität Darmstadt, Schlossgartenstraße 2, 64289 Darmstadt, Germany

²GSI Helmholtzzentrum für Schwerionenforschung, Planckstraße 1, 64291 Darmstadt, Germany

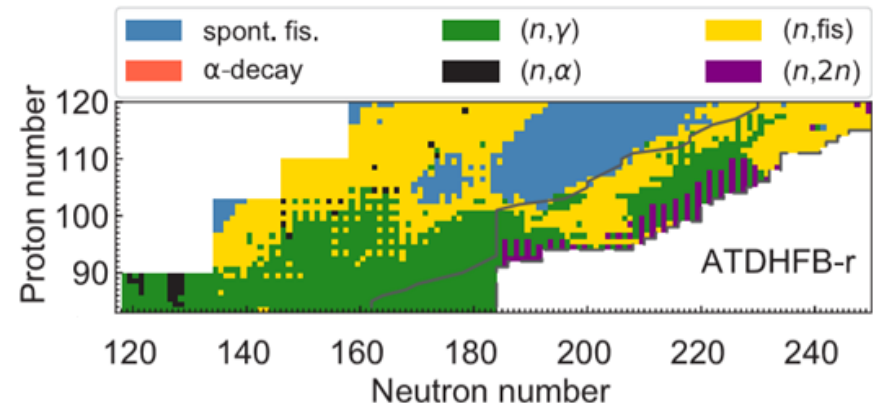
New BCPM EDF, Systematic calculations of fission ~ 3640 nuclei



Potential energy surface V

Collective inertia M

$$S = \int_{s_{\text{in}}}^{s_{\text{out}}} ds \sqrt{2\mathcal{M}(s)(V(s) - E)/\hbar^2}$$

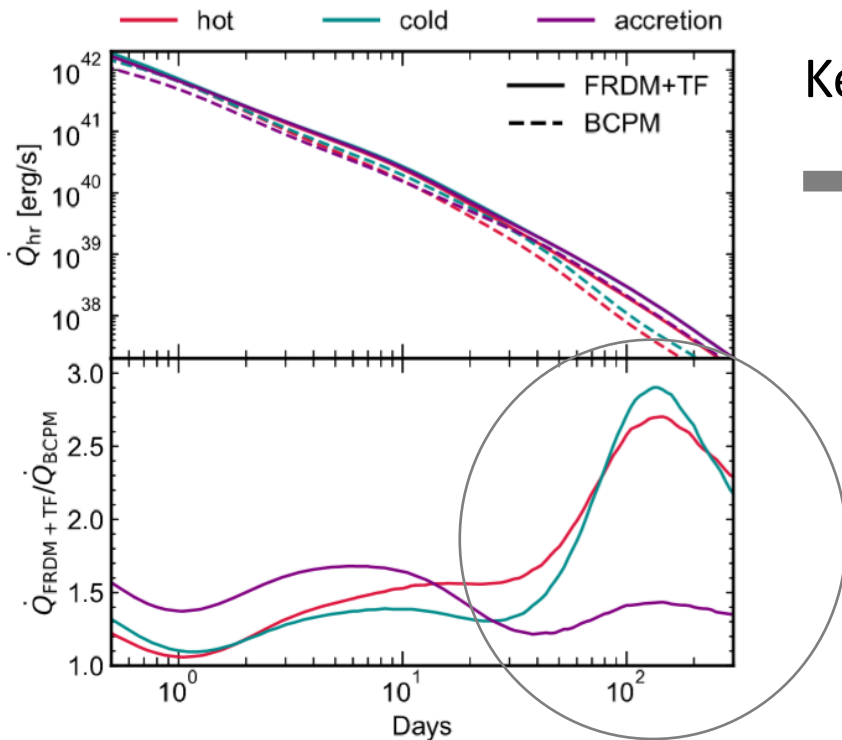
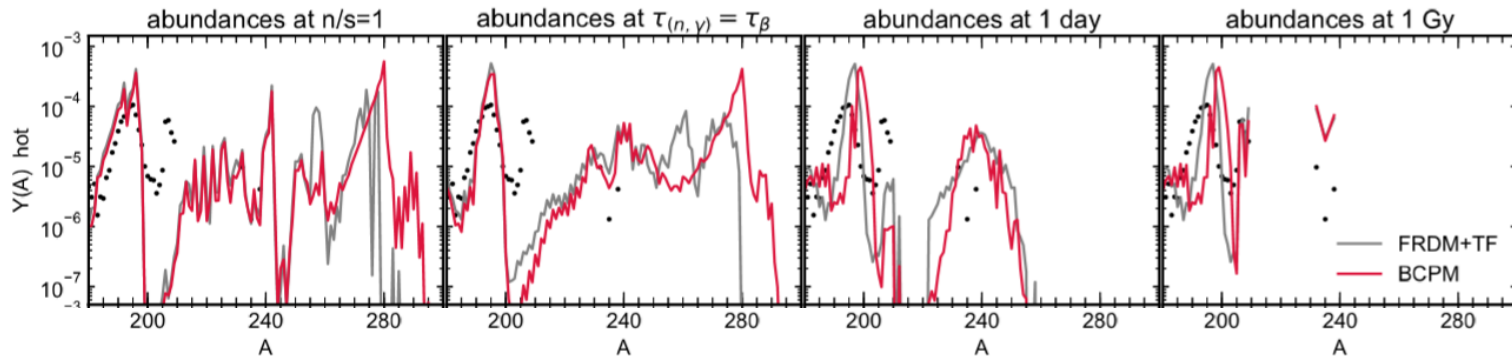


DFT-based r-process nucleosynthesis in NSM

Fission and the r -process nucleosynthesis of translead nuclei

arXiv:1904.03733

Samuel A. Giuliani,^{1,*} Gabriel Martínez-Pinedo,^{2,3,†} Meng-Ru Wu,^{4,5,‡} and Luis M. Robledo^{6,7,§}



Key nucleus ^{254}Cf , $T_{1/2}=60.5\text{d}$

➔ Kilonova lightcurve is sensitive to the amount of ^{254}Cf at $t > 10\text{--}100$ days

$A=280$ nuclei fission at $t < 1\text{day}$, producing neutrons, enhancing n -induced fission of $A=254$ nuclei

Ambiguity in spontaneous fission

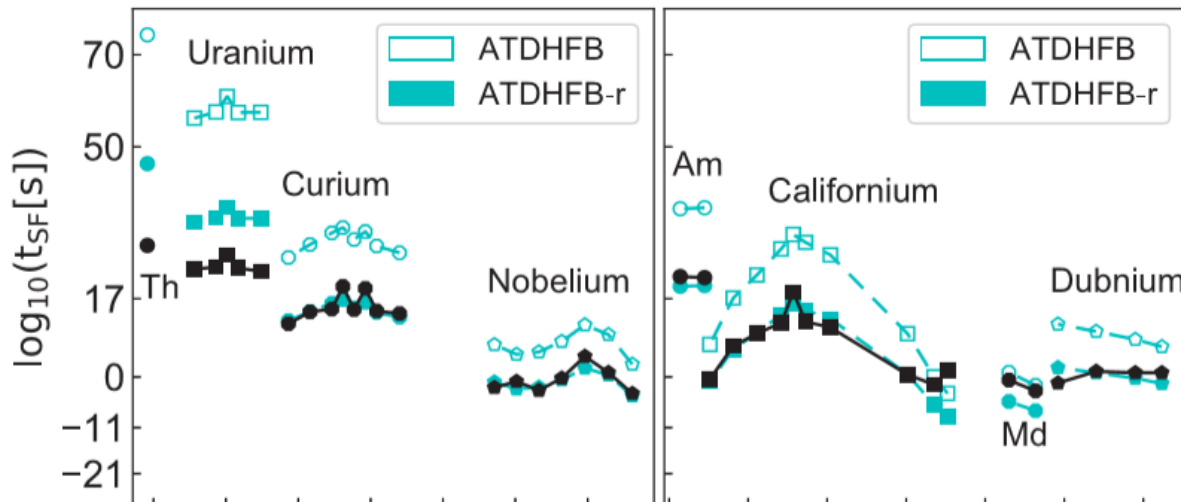
Sadhukhan et al, PRC88, 064314 (2013)

| Path | $S(L)$ | $\log_{10}(T_{1/2}/\text{yr})$ |
|--------------------------|--------|--------------------------------|
| DPM + \mathcal{M}^C | 19.1 | -11.4 |
| RM + \mathcal{M}^C | 18.9 | -11.6 |
| DPM + \mathcal{M}^{CP} | 16.8 | -13.4 |
| RM + \mathcal{M}^{CP} | 16.8 | -13.4 |

^{264}Fm ,

Difference of half lives
(order of magnitude)
with different models
for collective inertia

S.A. Giuliani et al, PRC97, 034323 (2018)



$$T_{\text{SF}}^{\text{th}} \gg T_{\text{SF}}^{\text{exp}}$$



Reduced collective
inertia (factor 0.5)

Formulation from Adiabatic TDHFB

Dobaczewski, Skalski, NPA369,123(1981)

- Little practical applications, inverse of huge QRPA matrix
- **Neglecting** dynamical residual interactions (Time-odd terms)
 - **Cranking approximation**
 - Practical use with recent DFT-based method

Formulation from Local QRPA

Hinohara et al., PRC82 (2010) 064313

- Approximation of adiabatic Self-consistent coordinate method
- Properly **including** residual interactions (Time-odd terms)
 - P + Q force, β - γ plane
Hinohara et al., PRC82 (2010) 064313, etc
 - Skyrme DFT, axial symmetry
Yoshida, Hinohara., PRC83 (2011) 061302

Motivation

Understand the origin of this fusion hindrance problem from microscopic point of view

Method

Local QRPA with Skyrme EDF to include dynamical residual effect to collective inertia

- Small computational cost
- Equivalent to QRPA response

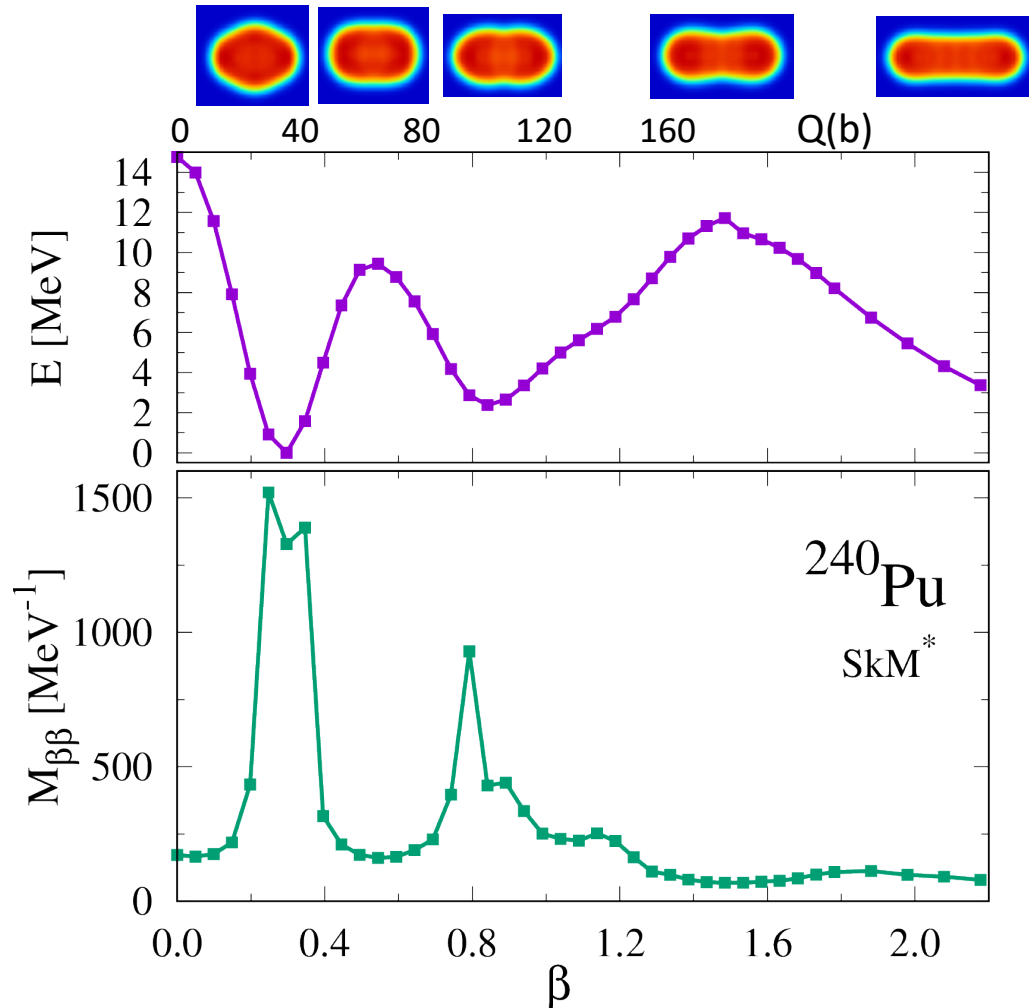
Nakatsukasa et al., PRC76 (2007) 024318
 Avogadro & Nakatsukasa, PRC84(2011)014314
 Stoitsov et al., PRC84 (2011) 041305
 Liang et al., PRC87 (2013) 054310
 Niksic et al., PRC88 (2013) 044327

| | 方程式 | 次元 | 解法 | cutoff |
|------|--|------------------|----------------------|-----------|
| FAM | $\begin{aligned} (E_\mu + E_\nu - \omega)X_{\mu\nu}(\omega) + \delta H_{\mu\nu}^{20}(\omega) &= -F_{\mu\nu}^{20} \\ (E_\mu + E_\nu + \omega)Y_{\mu\nu}(\omega) + \delta H_{\mu\nu}^{02}(\omega) &= -F_{\mu\nu}^{02} \end{aligned}$ | $N \times N$ | 反復法 | なし |
| QRPA | $\begin{pmatrix} A & B \\ -B^* & -A^* \end{pmatrix} \begin{pmatrix} X \\ Y \end{pmatrix} = \omega \begin{pmatrix} X \\ Y \end{pmatrix}$ | $N^2 \times N^2$ | 対角化 固有値 固有ベクトル | E_{2QP} |

N: Dimension of base($\sim 10^3$)

Result: Collective inertia along fission path

^{240}Pu Fission barrier, collective inertia $M_{\beta\beta}$



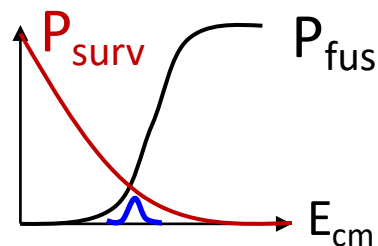
Large $M_{\beta\beta}$ at g.s. & fission isomer

Small $M_{\beta\beta}$ at large deformations

Sudden change of $M_{\beta\beta}$ around potential minima

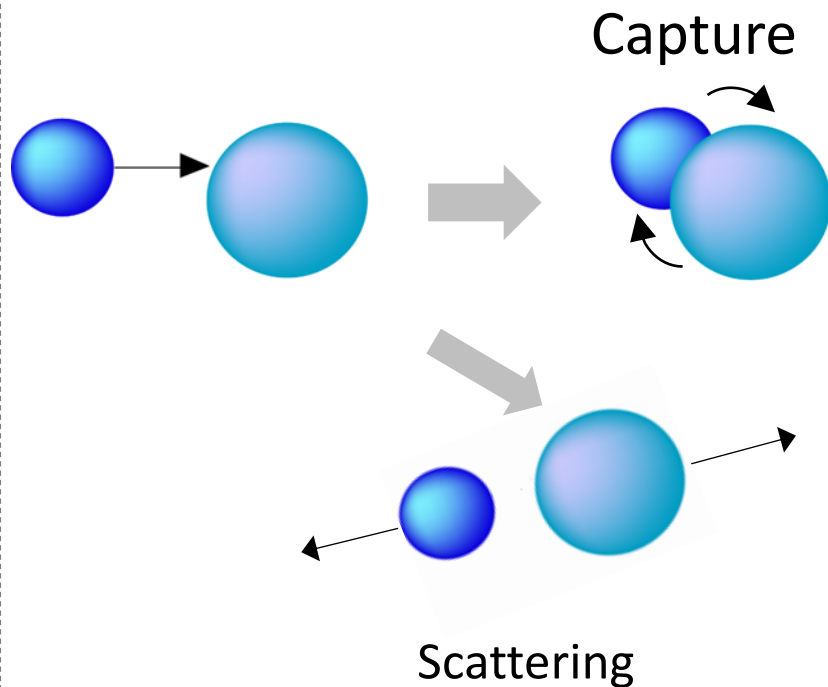
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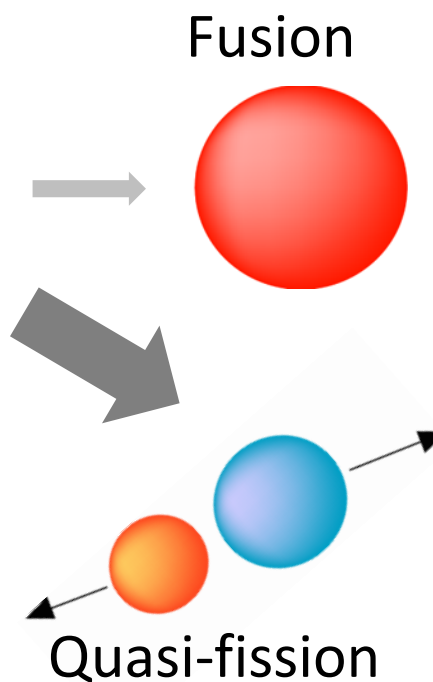


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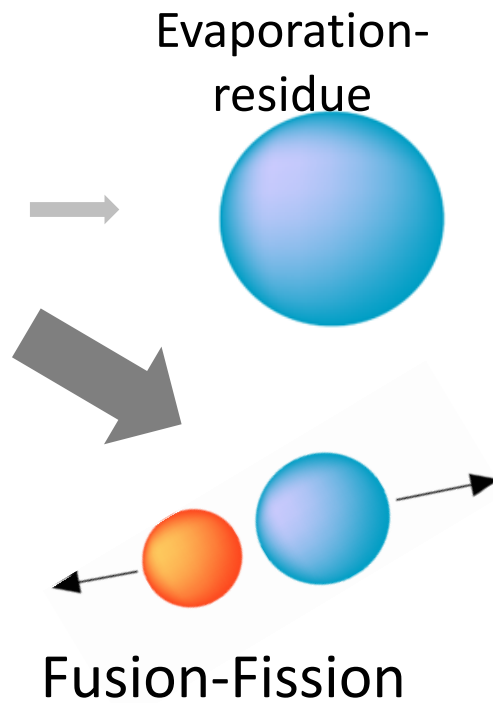
First stage



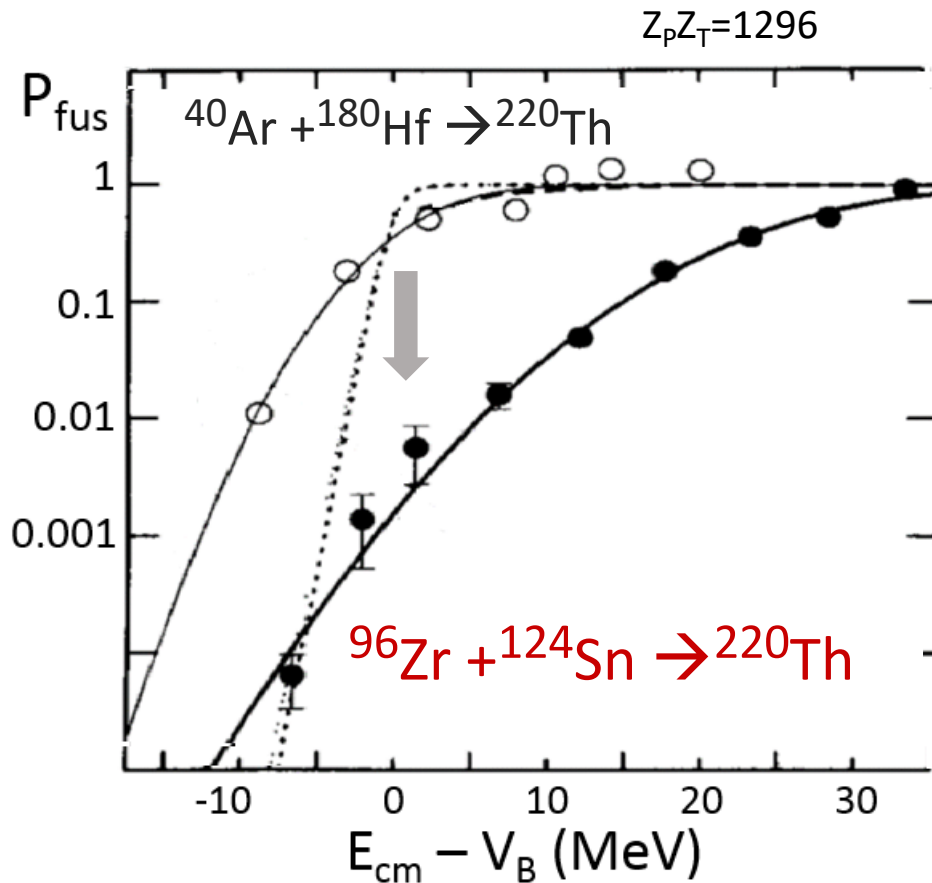
Second stage



Third stage

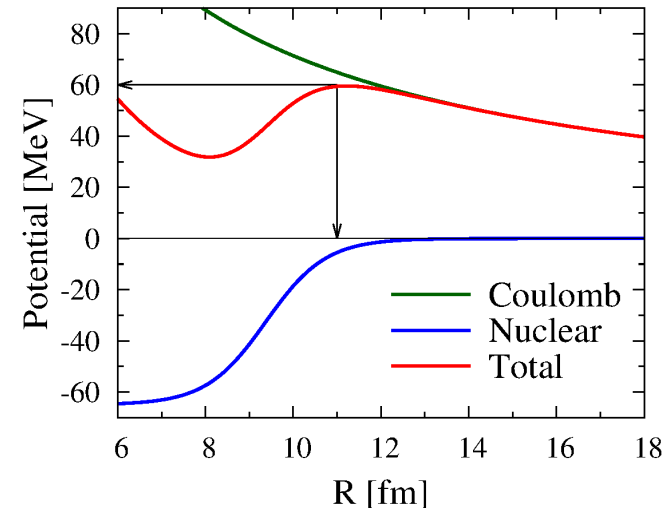


Fusion probability



V_B : Bass barrier

- Fusion probability is hindered in heavy systems ($Z_p Z_T > 1600$)
- Extra-push energy
Swiatecki, NPA376 (1982) 275
- Change in potential?
- Large energy dissipation?



Motivation

Understand the origin of this fusion hindrance problem from microscopic point of view

Method

Time-dependent density functional theory , TDDFT

(TDDFT)

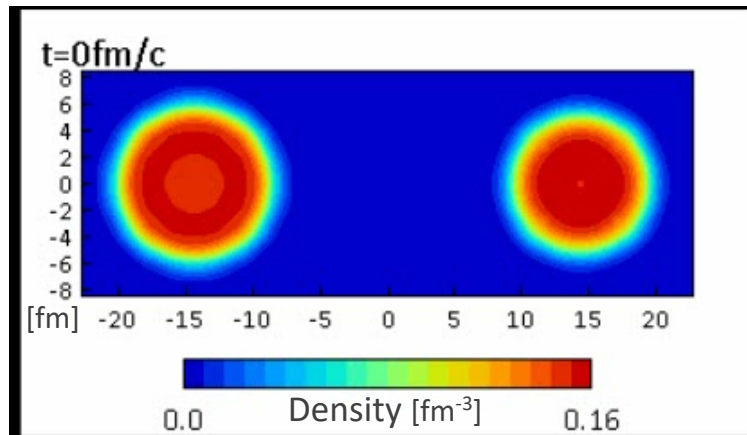
$$i\hbar \frac{\partial}{\partial t} \psi_i(\mathbf{r}, t) = \hat{h}[\rho(\mathbf{r}, t)] \psi_i(\mathbf{r}, t)$$

$^{96}\text{Zr} + ^{124}\text{Sn}$

Central collision

$E_{\text{cm}} = 225 \text{ MeV}$

$V_B \sim 214 \text{ MeV}$



Bonche et al., PRC13 (1976)
Flocard et al., PRC17 (1978)
Negele, RMP54 (1982)
Kim et al., J. Phys. G23 (1997)
Simenel et al., PRL86 (2001)
Nakatsukasa, Yabana, PRC71(2005)
Umar, Oberacker, PRC73 (2006)
Avez et al., PRC78 (2008)
Ebata et al., PRC82 (2010)
Stetcu et al., PRC84 (2011)

$$\rho(\mathbf{r}, t) = \sum_{i=1}^N |\psi_i(\mathbf{r}, t)|^2$$

- Same description on **structure** and **dynamics**
- No phenomenological parameters for **dynamics**
- Single-particle: **quantum**, Relative motion: **classical**

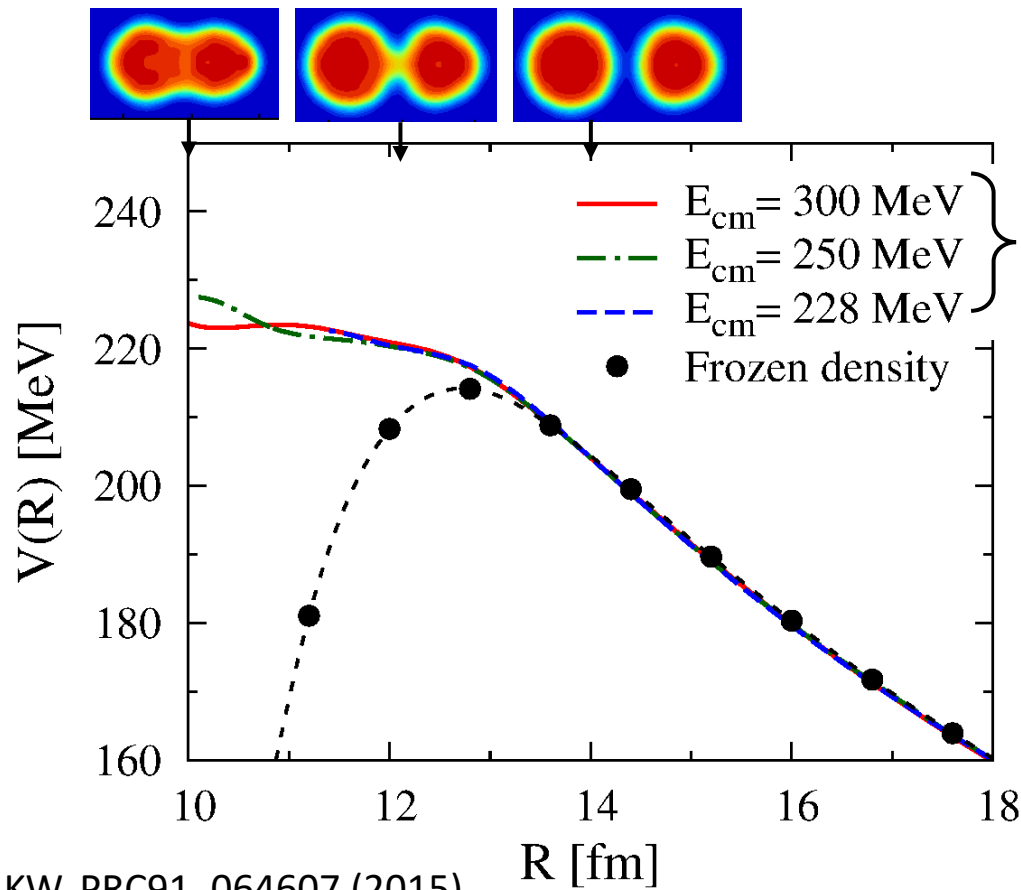
Result: Nucleus-nucleus potential

TDDFT (microscopic) $\rightarrow \frac{dP}{dt} = -\frac{dV(R)}{dR} - \frac{d}{dR} \frac{P^2}{2\mu(R)} - \gamma(R) \frac{dR}{dt}$

$^{96}\text{Zr} + ^{124}\text{Sn}$ potential

KW, Lacroix, PRC78(2008)024610

KW, Lacroix, Ayik, PRC79(2009)

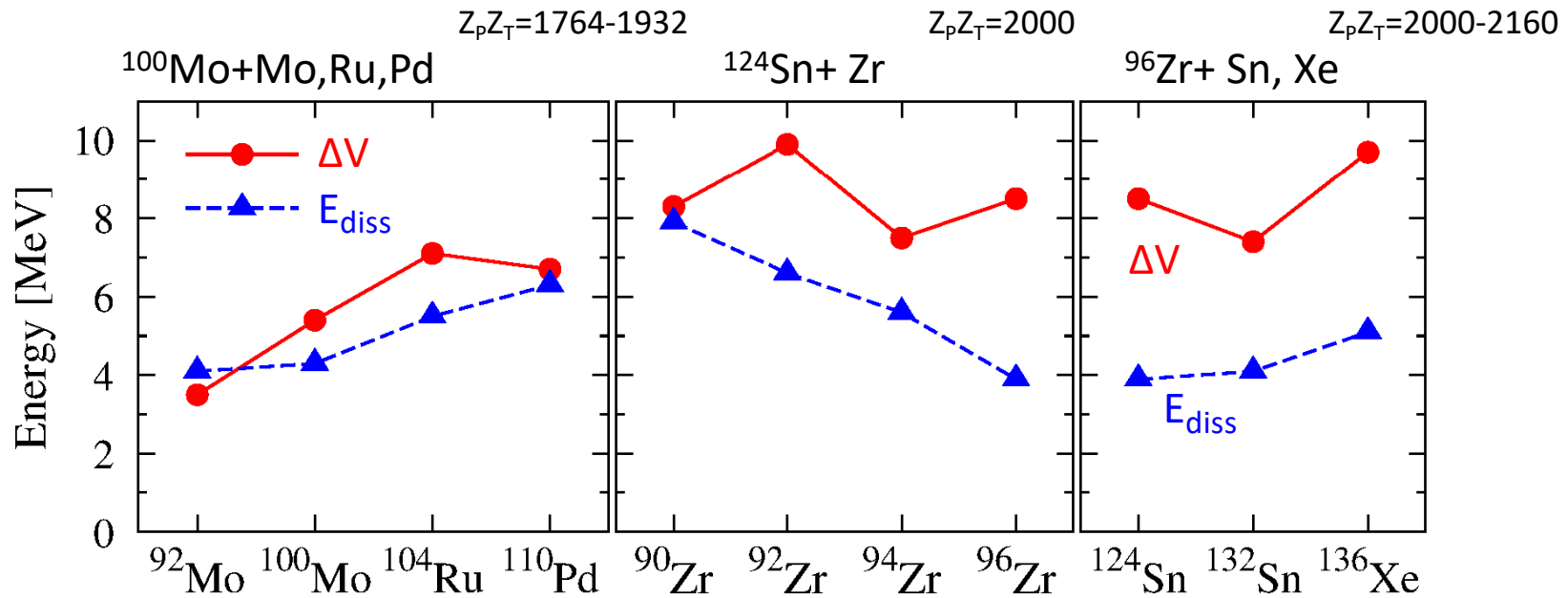


TDDFT

- No barrier
- Small energy dependence

Origin of fusion hindrance

$$E_{\text{extra}} = \text{increase in potential } (\Delta V) + \text{dissipated energy } (E_{\text{diss}})$$



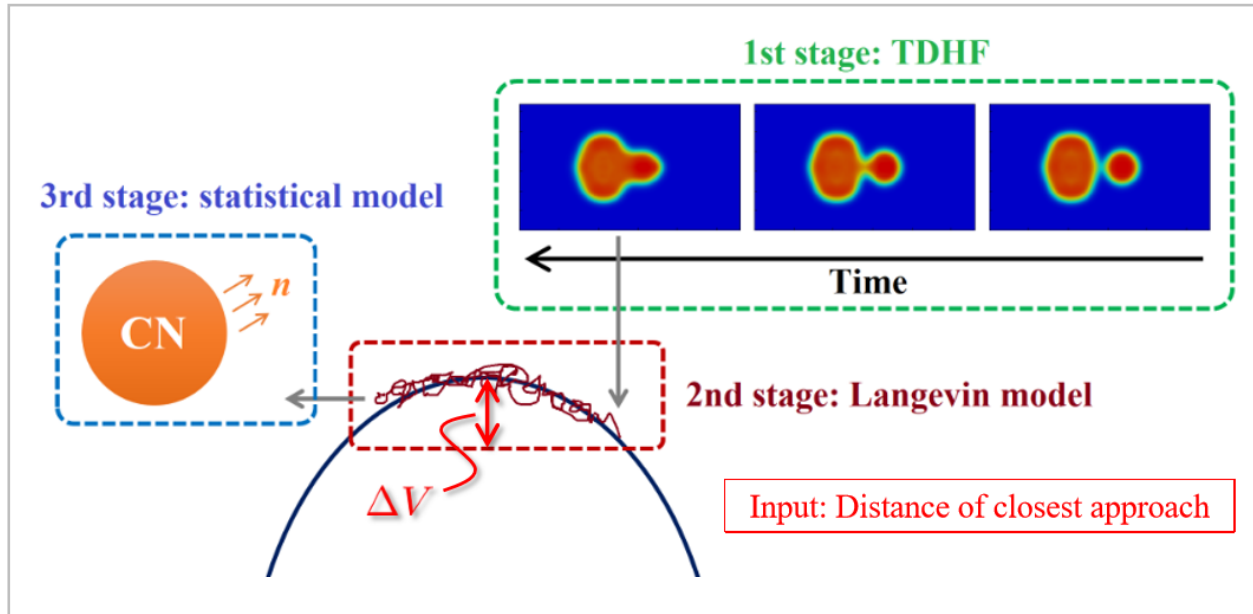
$$\Delta V > E_{\text{diss}}$$

Origin of fusion hindrance is a dynamical increase in potential ΔV at small R

Hybrid model of SHE formation

Sekizawa, Hagino, PRC99, 051602(R) (2019)

Editors' Suggestions



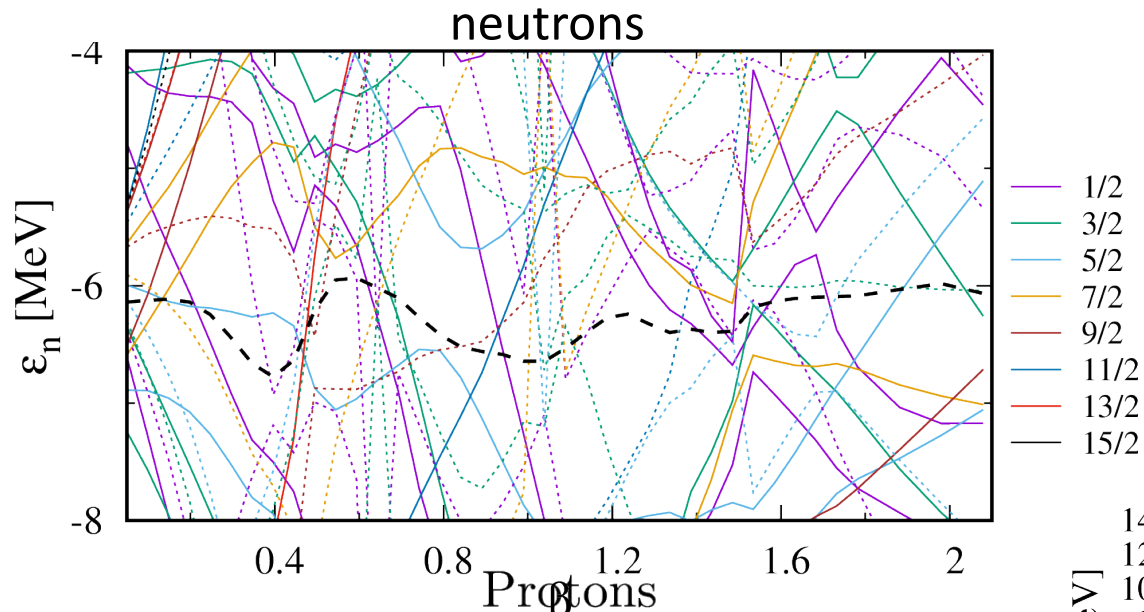
TDDFT + Langevin +
Statistical model

| System | CN | E^* (MeV) | TDHF | FBD | W_{sur} ($\times 10^9$) | $P_{\text{CN}} W_{\text{sur}}$ ($\times 10^{13}$) |
|------------------------------------|----------------|----------------|--------------------------|--------------------------------------|---------------------------------------|--|
| | | | R_{min} (fm) | P_{CN} ($\times 10^4$) | | |
| $^{48}\text{Ca} + ^{254}\text{Fm}$ | $^{302}_{120}$ | 29.0 | 12.93 | 1.72 | 176 | 302 |
| $^{54}\text{Cr} + ^{248}\text{Cm}$ | $^{302}_{120}$ | 33.2 | 13.09 | 1.89 | 1.31 | 2.47 |
| $^{51}\text{V} + ^{249}\text{Bk}$ | $^{300}_{120}$ | 37.0 | 12.94 | 3.95 | 0.117 | 0.461 |
| $^{48}\text{Ca} + ^{257}\text{Fm}$ | $^{305}_{120}$ | 30.5 | 12.94 | 2.49 | 0.729 | 1.82 |

Shell effect of ^{48}Ca
affects the probability in
the third stage

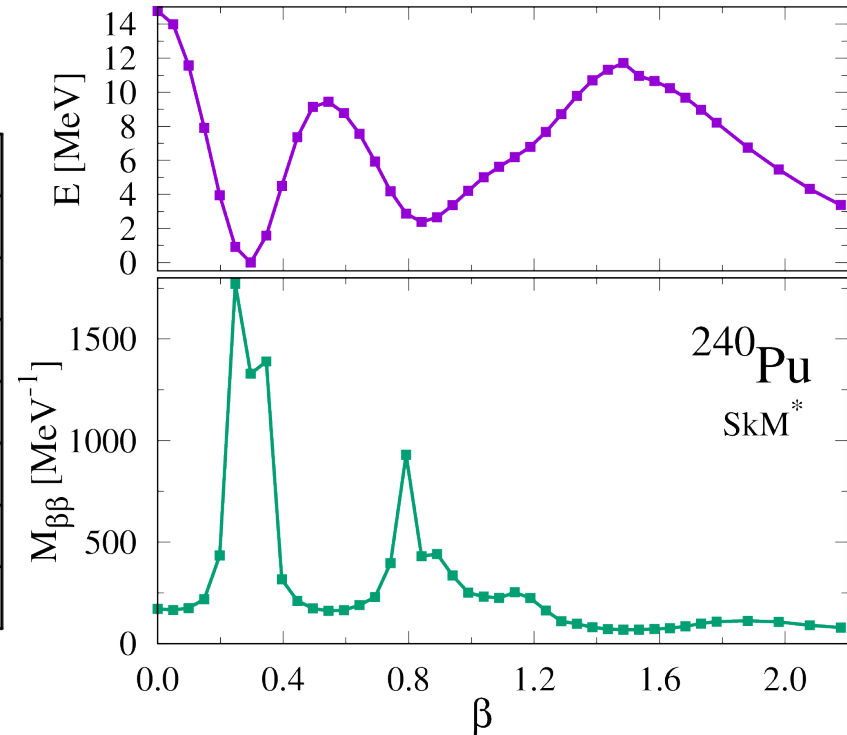
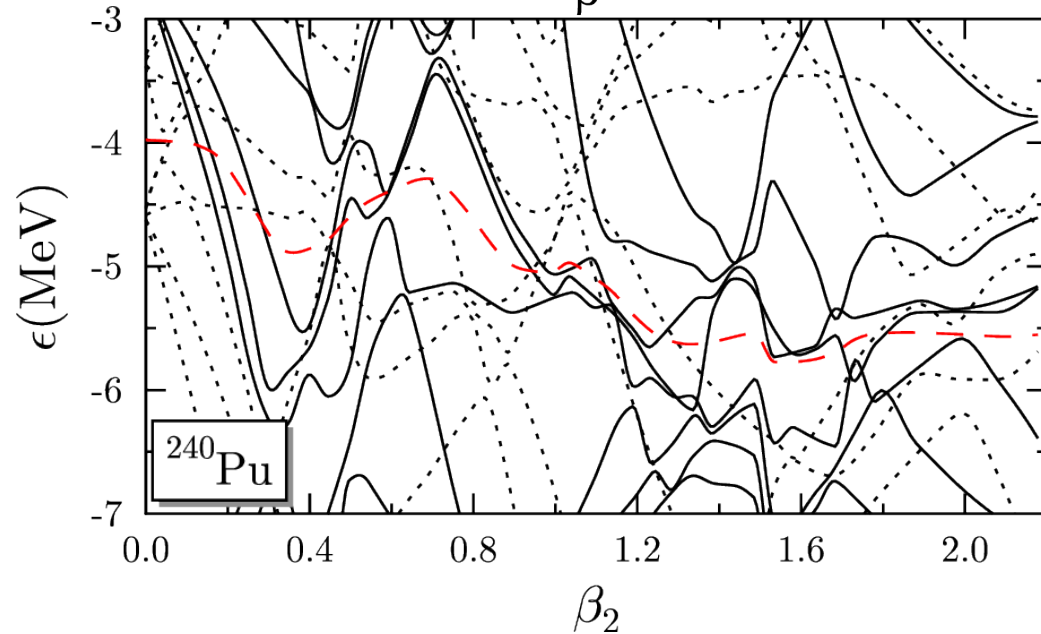
- 超重元素の性質、多様な崩壊形式、殻効果で安定化
- 超重元素生成、競合過程
- Fission is a dominant mode against SHE synthesis
- Fission is relevant to r-process nucleosynthesis
- ^{254}Cf is a key nucleus for kilonova lightcurves at $t > 10\text{-}100\text{days}$
- Ambiguity in fission: Collective inertia
 - Local QRPA approach to include dynamical effect
- Fusion hindrance problem analyzed by TDDFT
 - Dynamical effect of potential increase is a main origin of this hindrance

核分裂経路での質量と一粒子準位



Mass が急激に変化する
 $\beta=0.4, 0.7$ で level crossing

一方 $\beta=1.0, 1.4$ では mass に
 大きな変化なし。

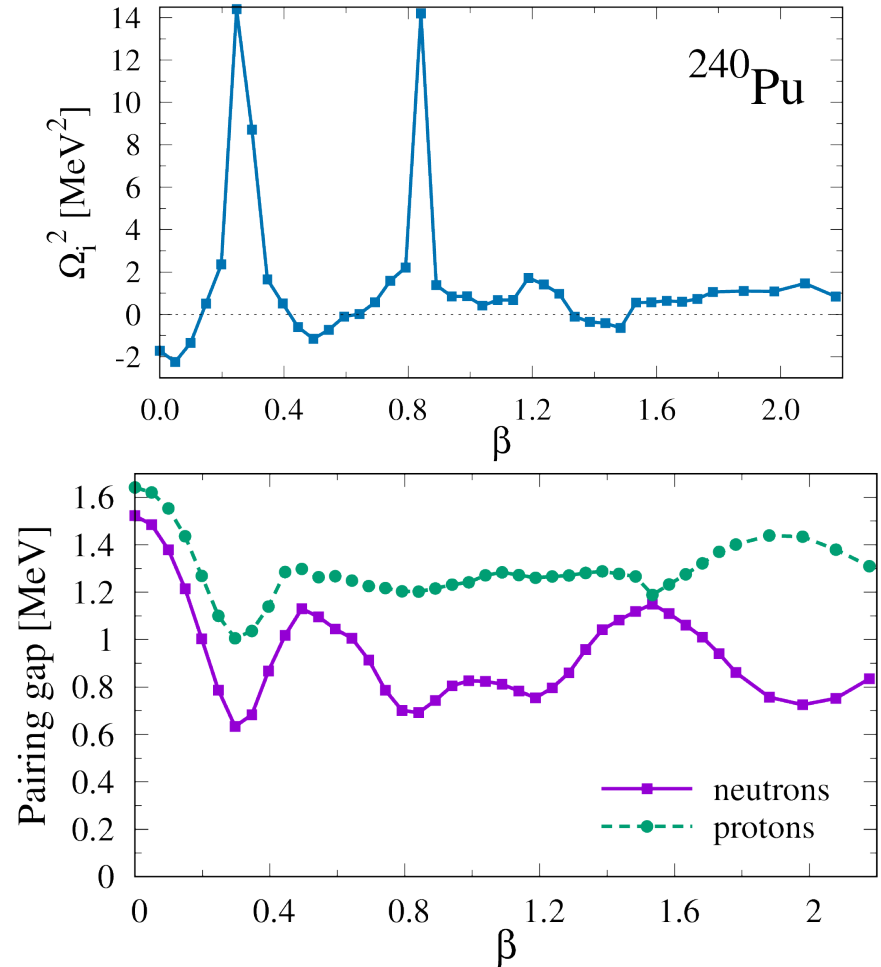
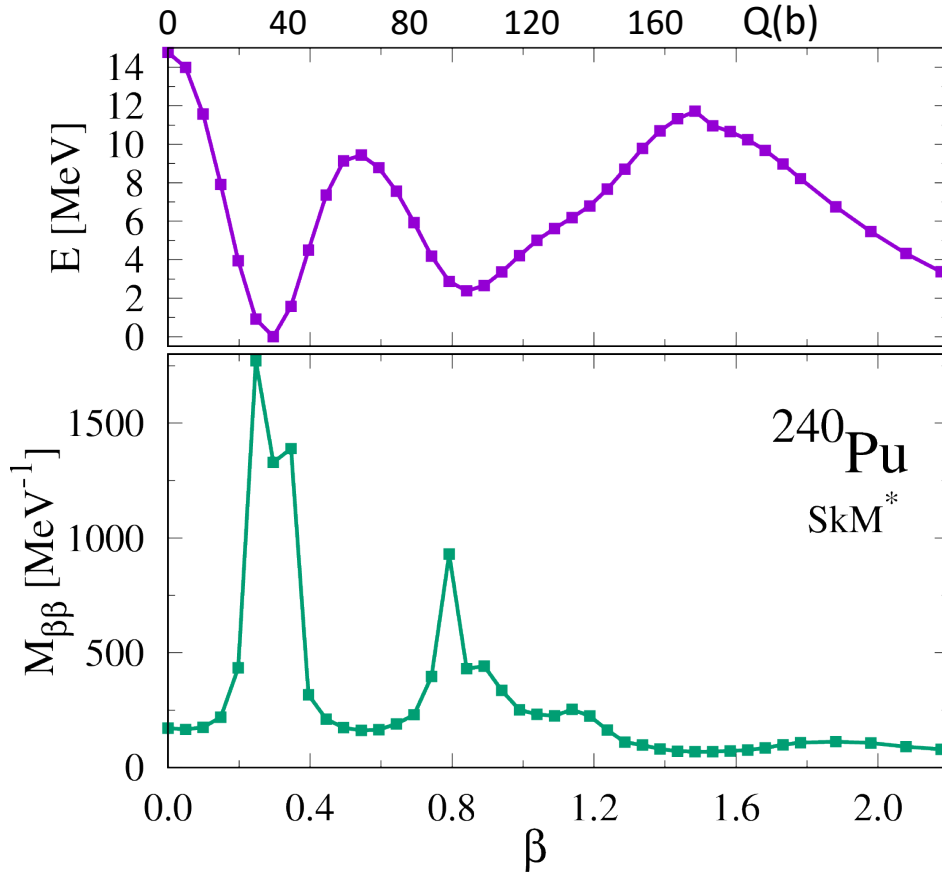


核分裂経路での質量 (β 自由度のみ)

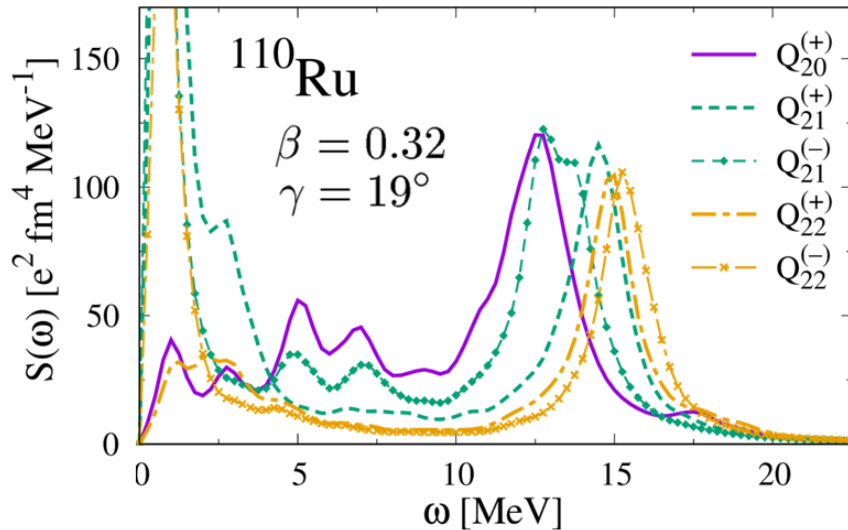
外場 : Isoscalar Q_{20}

$\Omega_i < 4$ MeV で最も集団的なモード = 最大の $|\langle P_i | \hat{Q}_{20} | 0 \rangle|$ を選択

^{240}Pu 核分裂障壁と質量 $M_{\beta\beta}$

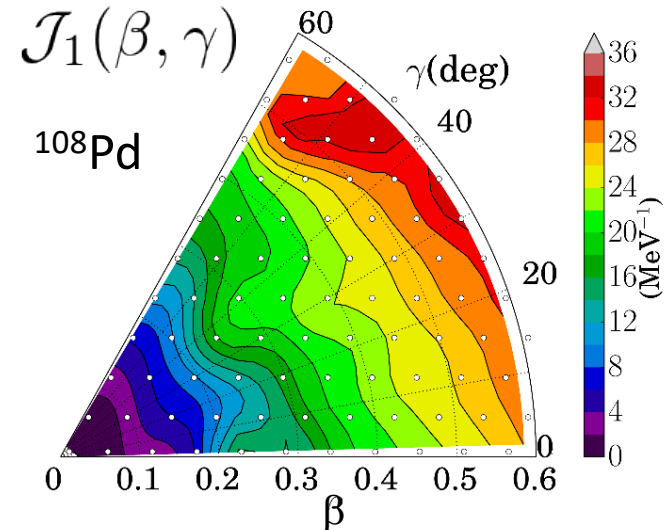


アイソスカラー型四重極強度関数



$$S(\hat{F}, \omega) = -\frac{1}{\pi} \text{Im} \left(\sum_{\mu < \nu} F_{\mu\nu}^{20*} X_{\mu\nu}(\omega) + F_{\mu\nu}^{02*} Y_{\mu\nu}(\omega) \right)$$

回転に対する慣性モーメント



$$S^{\text{FAM}}(\hat{F} = \hat{J}_k, \omega = 0) = -\mathcal{J}_k$$

- 密度汎関数法に基づく非軸対称核の線形応答計算
- 短いCPU時間で計算実行可能

~15 min/ ω (16threads), 3.5 GB memory

Numerical set up

$^{110}\text{Ru}, ^{108}\text{Pd}$: 17^3 mesh, $R_{\text{max}}=14.0\text{fm}$, $N_{\text{base}}=1120$

KW, Nakatsukasa, PRC96, 041304(R) (2017)

KW, Nakatsukasa, JPS Conf. Proc. 23, 013012 (2018)

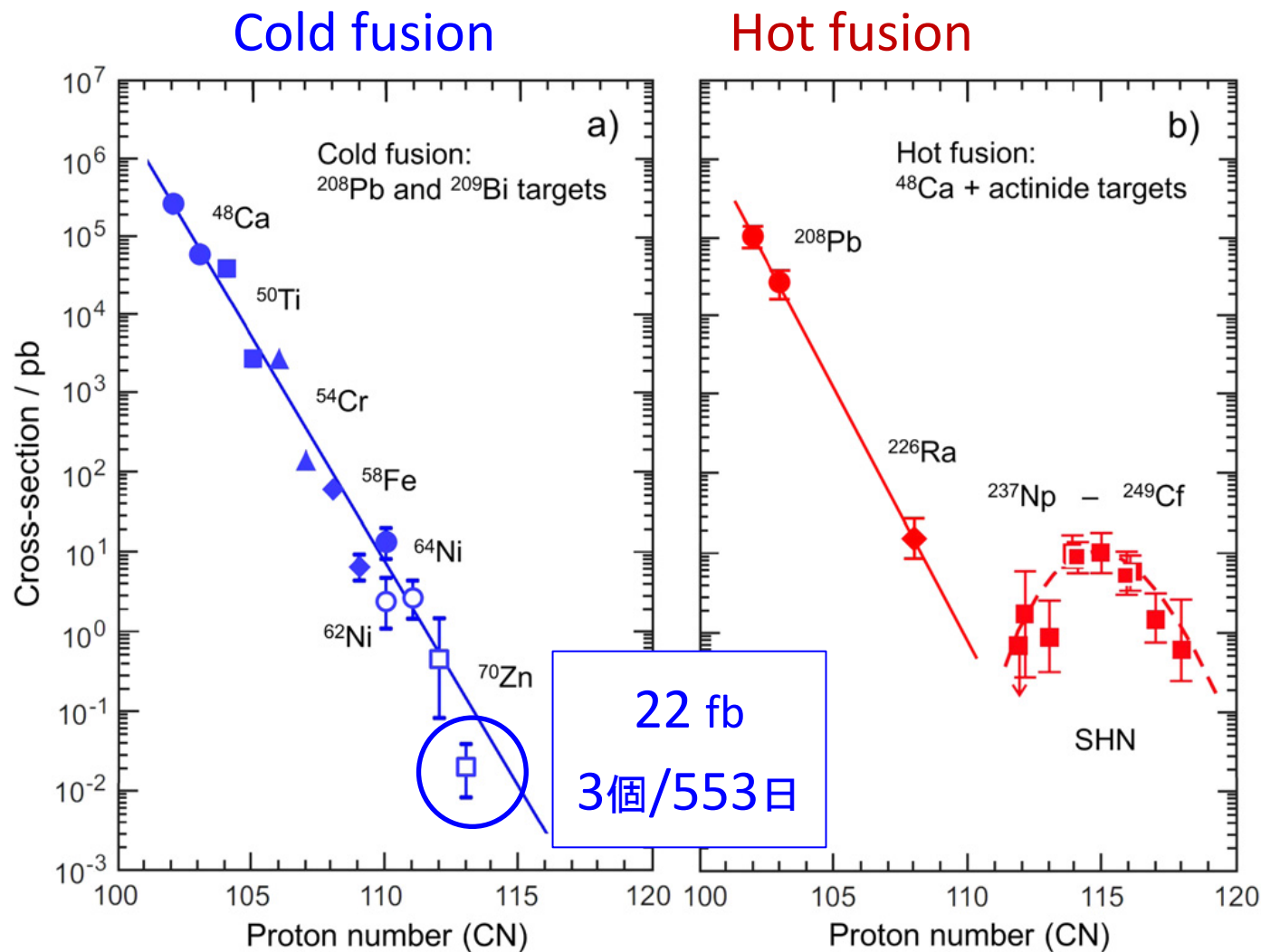
$$E_0 = \min_{\rho} E[\rho]$$

$$E = T_0 + E^{\text{s.o.}} + E_{\text{int}}^{\infty} + E_{\text{int}}^{\text{FR}} + E_C.$$

$$E_{\text{int}}^{\text{FR}}[\rho_n, \rho_p] = \frac{1}{2} \sum_{t,t'} \iint d\mathbf{r} d\mathbf{r}' \rho_t(\mathbf{r}) v_{t,t'}(\mathbf{r} - \mathbf{r}') \rho_{t'}(\mathbf{r}') \\ - \frac{1}{2} \sum_{t,t'} \gamma_{t,t'} \int d\mathbf{r} \rho_t(\mathbf{r}) \rho_{t'}(\mathbf{r}),$$

$$E_{\text{int}}^{\infty}[\rho_p, \rho_n] = \int d\mathbf{r} [P_s(\rho)(1 - \beta^2) + P_n(\rho)\beta^2] \rho \\ P_s(\rho) = \sum_{n=1}^5 a_n \left(\frac{\rho}{\rho_0} \right)^n, \quad P_n(\rho) = \sum_{n=1}^5 b_n \left(\frac{\rho}{\rho_{0n}} \right)^n$$

Introduction: Superheavy element research



安定の島に
近づいている？