Study of five-dimensional potential-energy surfaces for actinide isotopes in the double center oscillator model

Presented by Zhiming Wang

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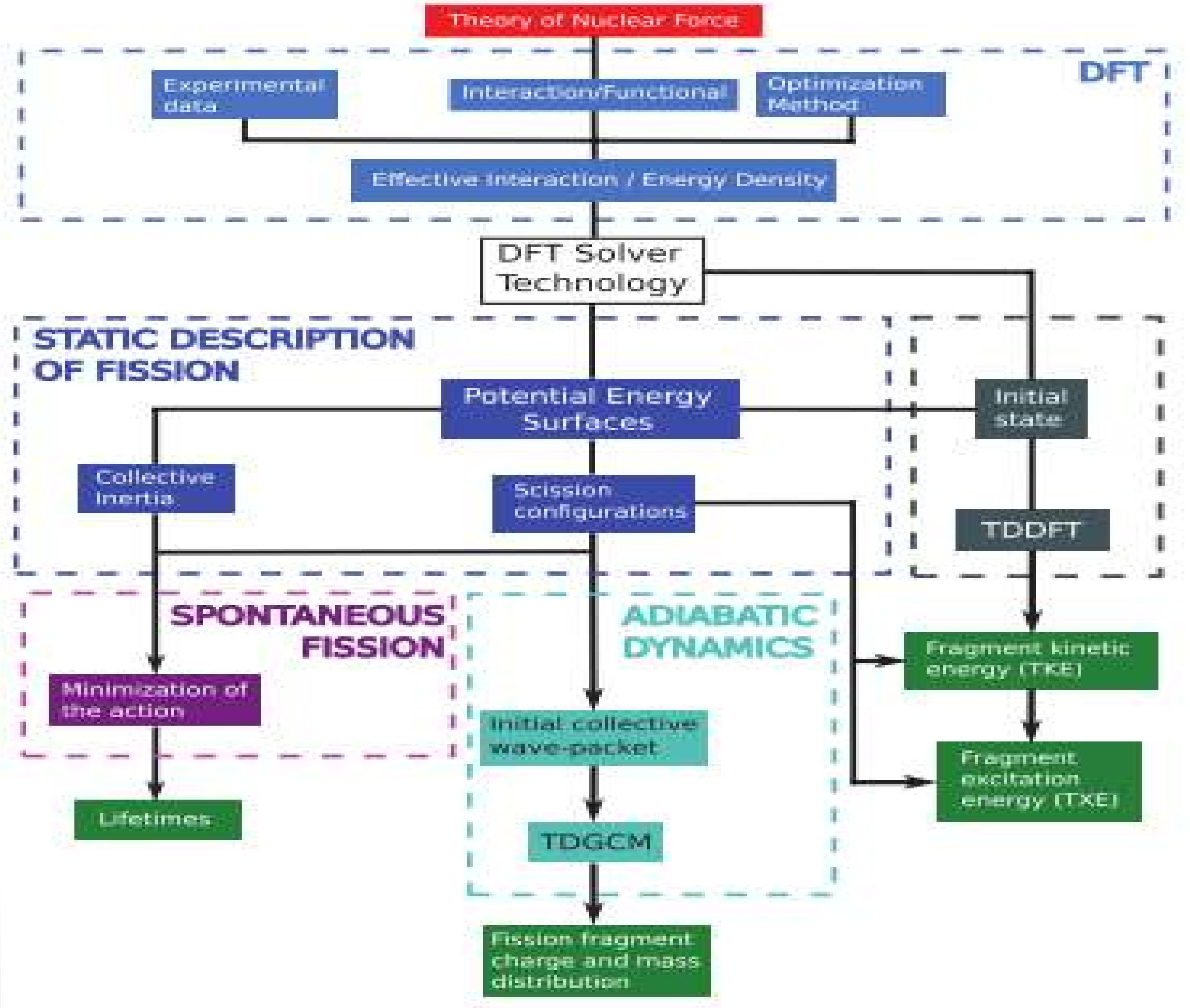
- **Background**
- Calculation of 5D PES
- Height of Fission Barriers
- Summary

Microscopic method



Theory of Nuclear Force

DFT

Experimental data

Interaction/Functional

Optimization Method

Effective Interaction / Energy Density

DFT Solver Technology

STATIC DESCRIPTION OF FISSION

Potential Energy Surfaces

Collective Inertia

Scission configurations

Initial state

TDDFT

SPONTANEOUS FISSION

Minimization of the action

Lifetimes

ADIABATIC DYNAMICS

Initial collective wave-packet

TDGCM

Fission fragment charge and mass distribution

Fragment kinetic energy (TKE)

Fragment excitation energy (TXE)

N. Schunck and L. M. Robledo,
Reports Prog. Phys. **79**, 116301 (2016).

Background

- **Macroscopic-Microscopic (MM) Model**

Three main parts in the MM model to calculate PES

- **Shape description**

  Shape description should be able to describe all the possible shape from spheroid (ground-state) to the dumbbell-like shape

- **Macroscopic energy**

  Macroscopic energy should be able to use for large deformation.

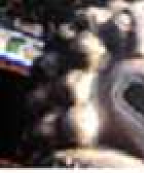
- **Microscopic energy**

  Microscopic energy should be precise enough.

Both macroscopic energy and microscopic energy are shape dependent.

Static analysis: barriers and fission path

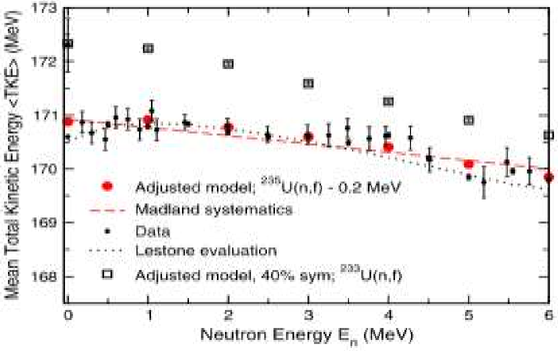
Post-fission phenomena obtained from dynamic calculations based on the PES.

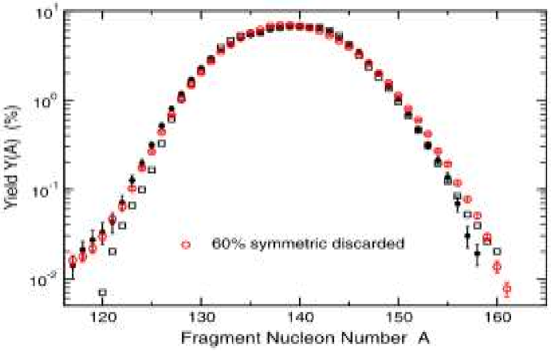


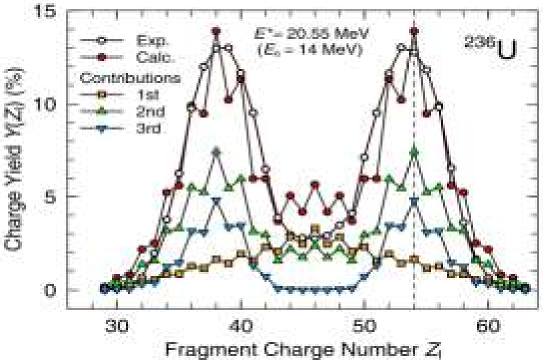
MM Model

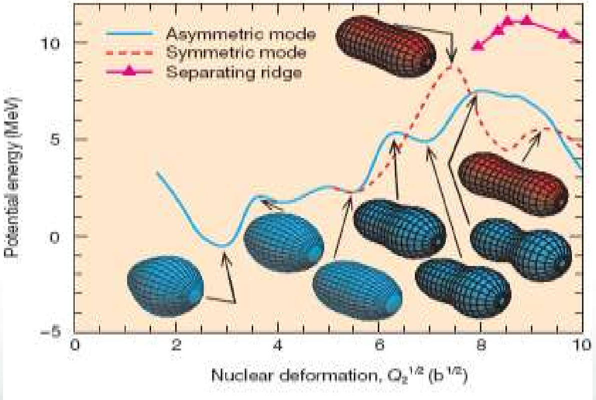
P. Möller et al.

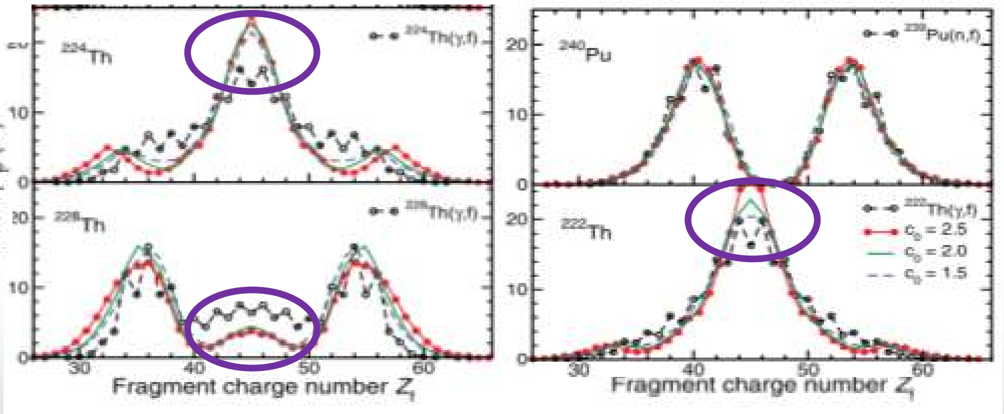
Shape description	Macroscopic energy	Microscopic energy
[redacted]	[redacted]	[redacted]





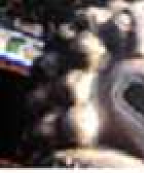






Physical Review C, (2009), 79(6), 064304.
P. Möller et al., Nature 409 (2001)785

Randrup, J., et al. Physical Review C, 84(3), 34613,
Physical Review Letters, 106(13), 132503.



MM Model

S. Chiba et al.

Shape description	Macroscopic energy	Microscopic energy
[redacted]		

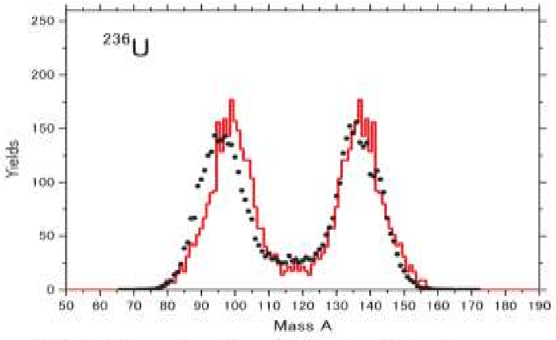


FIG. 4. (Color online) Mass distribution of fission fragments of ^{236}U at E^* = 20 MeV. Calculation and experimental data are denoted by histogram and circles, respectively.

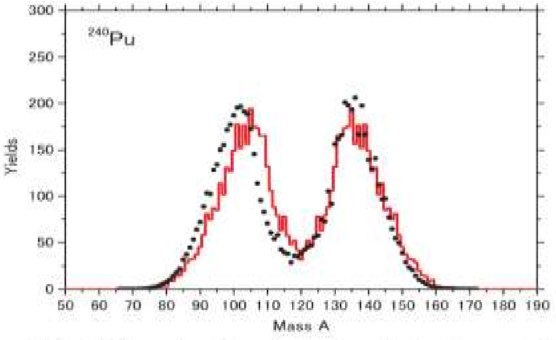
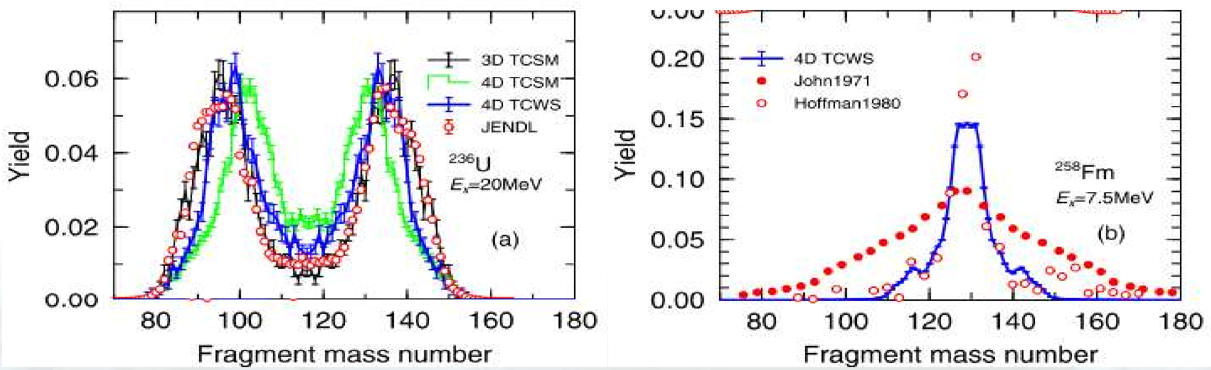
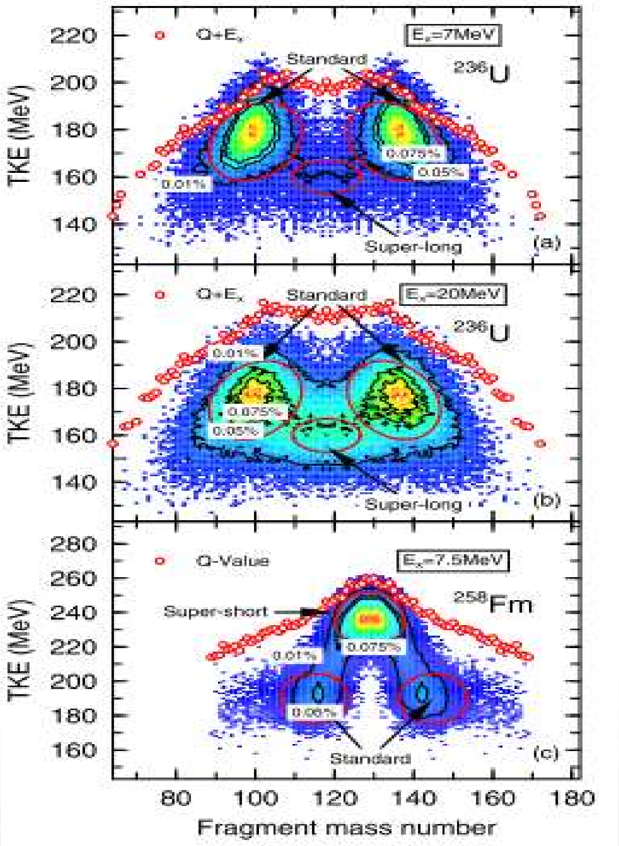


FIG. 6. (Color online) Mass distribution of fission fragments of ^{240}Pu at E^* = 20 MeV. Calculation and experimental data are denoted by histogram and circles, respectively.

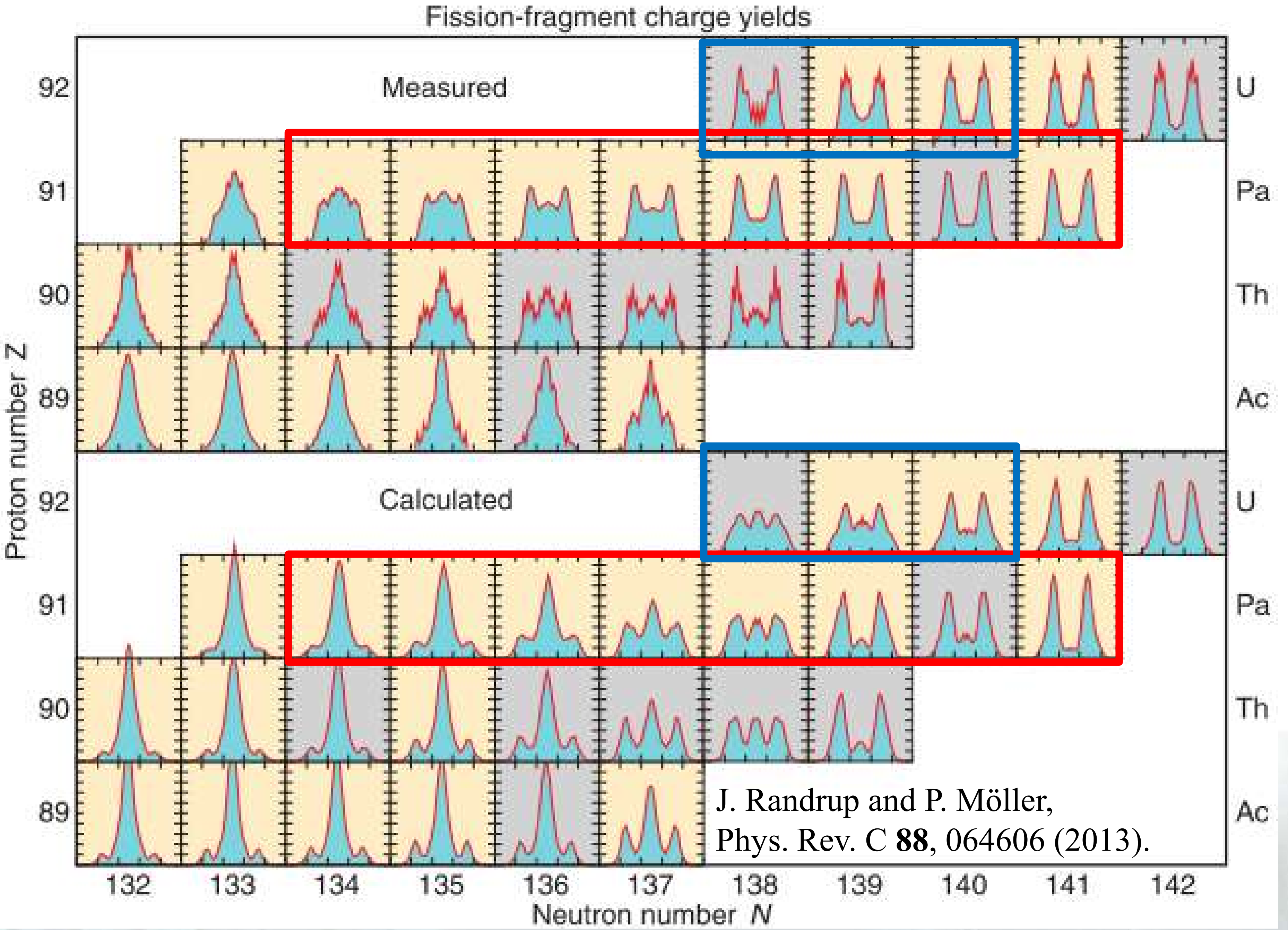




Aritomo, Y. et al, Phys. Rev. C 88(4), 1–7 (2013).

M. D. Usang et al, Phys. Rev. C ***96****, 64617 (2017).*

J. Maruhn and W. Greiner, Zeitschrift Für Phys. **251**, 431 (1972).

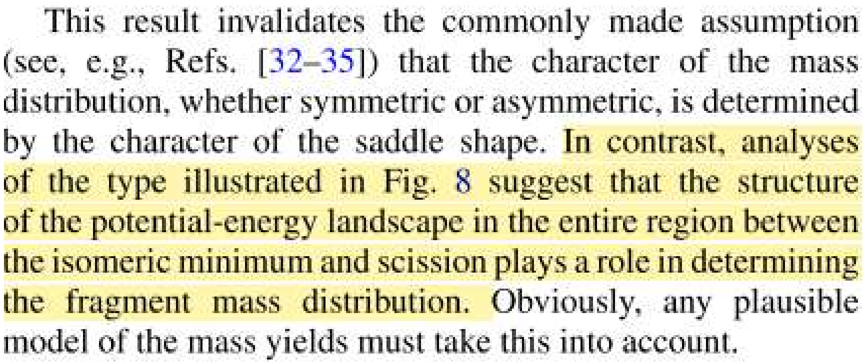


J. Randrup and P. Möller,
Phys. Rev. C **88**, 064606 (2013).

Background—Double Center Model

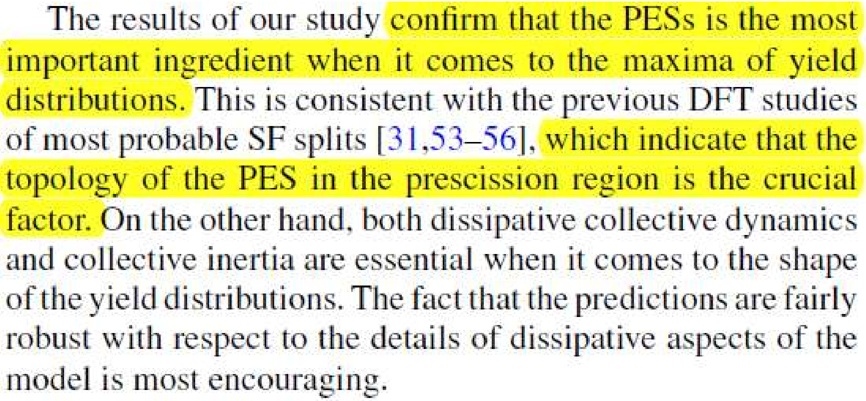
Why double center model?

more and more researchers have realized that the topology of the region between the fission barrier and scission has important influence on the fission fragment mass distribution. So a precise value of this region can help produce consistent results with the experiments.



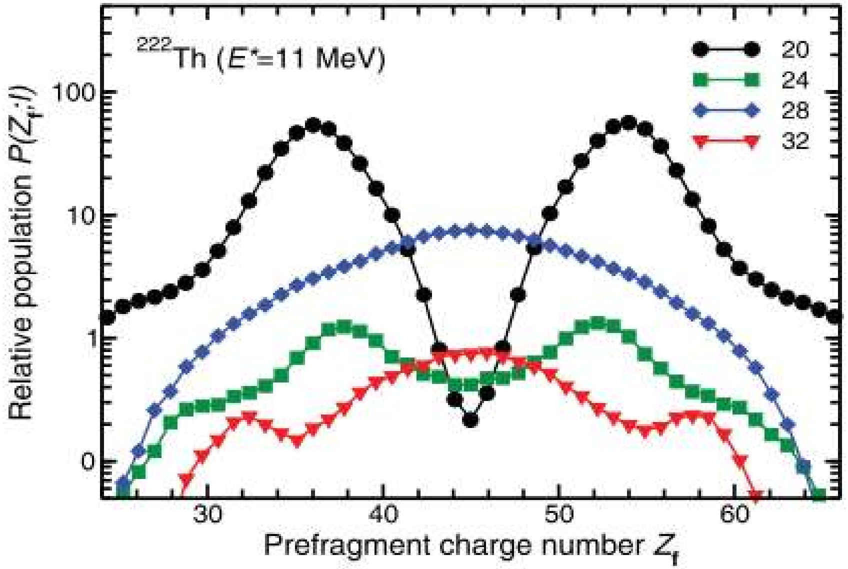
This result invalidates the commonly made assumption (see, e.g., Refs. [32–35]) that the character of the mass distribution, whether symmetric or asymmetric, is determined by the character of the saddle shape. In contrast, analyses of the type illustrated in Fig. 8 suggest that the structure of the potential-energy landscape in the entire region between the isomeric minimum and scission plays a role in determining the fragment mass distribution. Obviously, any plausible model of the mass yields must take this into account.

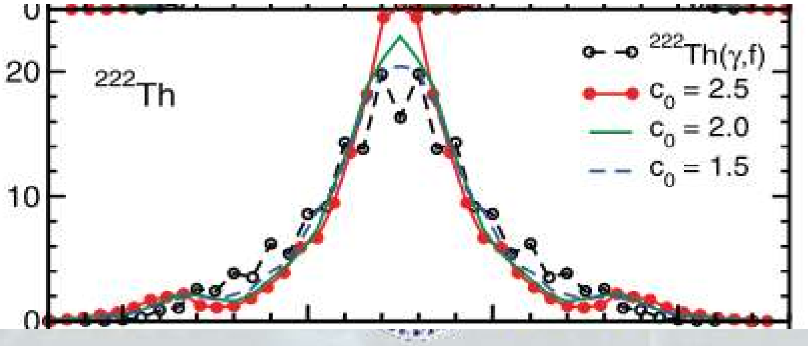
Phys. Rev. C, 84(3), 034613. (2011).



The results of our study confirm that the PESs is the most important ingredient when it comes to the maxima of yield distributions. This is consistent with the previous DFT studies of most probable SF splits [31,53–56], which indicate that the topology of the PES in the prescission region is the crucial factor. On the other hand, both dissipative collective dynamics and collective inertia are essential when it comes to the shape of the yield distributions. The fact that the predictions are fairly robust with respect to the details of dissipative aspects of the model is most encouraging.

Phys. Rev. C **93**, *011304(R) (2016)*

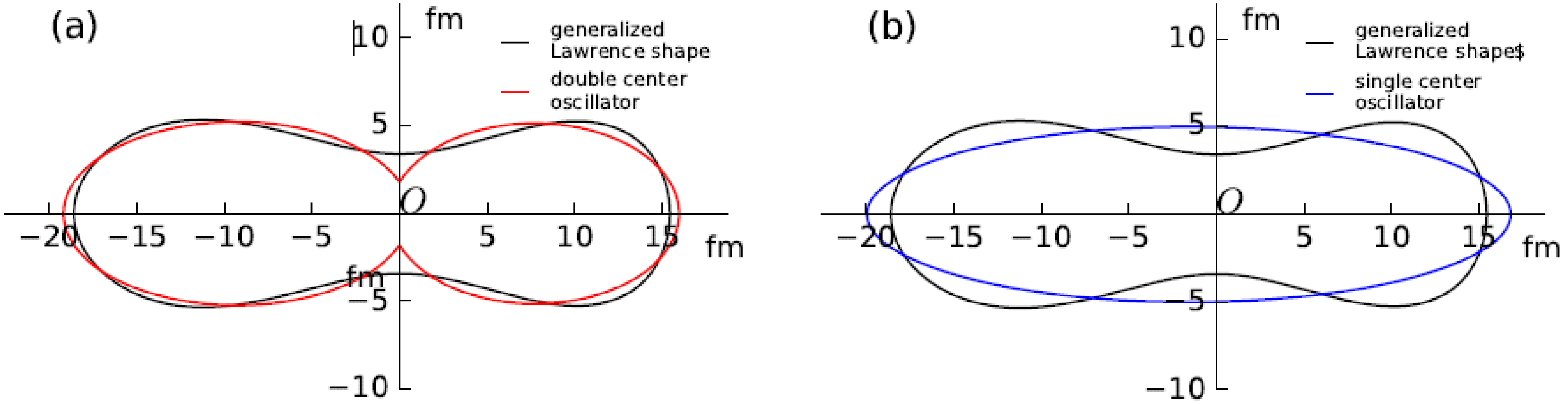




Background—Double Center Model

Why double center model?

Double center model can improve the calculation of energy levels and, furthermore, improve the microscopic correction energy



Theoretically, any kind of normalized, orthogonal and complete bases can be used to obtain the real energy levels of the deformed nucleus. However, the computer cannot use the infinite bases to obtain the realistic bases. Finite number of bases will introduce the truncation error in the calculation of energy levels.

Closer shape between the realistic bases and the double center model bases can reduce the truncation error.

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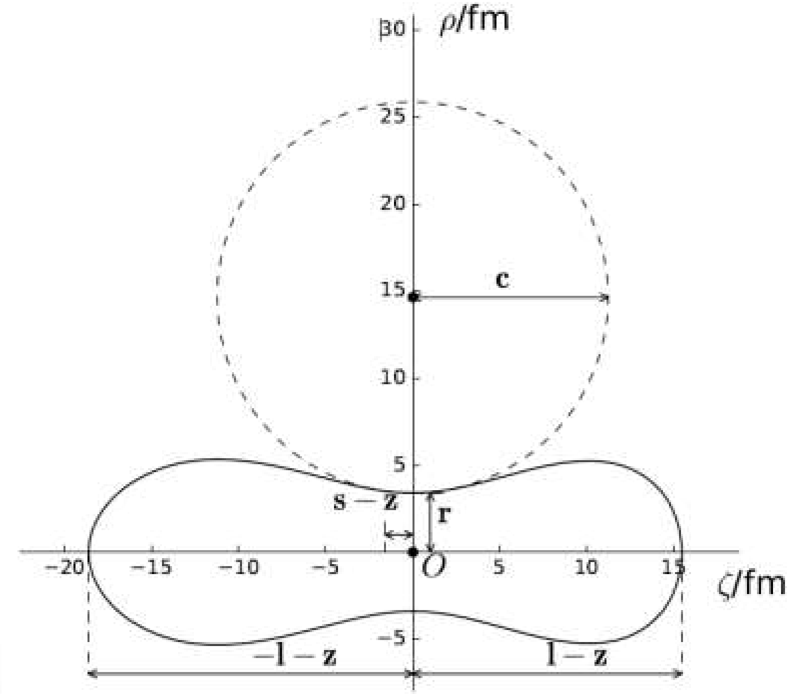
5D PES calculation

Shape description—generalized Lawrence shape (GLS)

- l, r, z, c and s
- total grid number: 30×32×26×26×21 = 13,628,160



J. Lawrence, Phys. Rev. 139(1965) B1227
U. Brosa, S. Grossmann, and A. Muller, Phys. Rep. 197 (1990) 167.

5D PES calculation

Macroscopic energy—Lublin-Strasbourg Drop (LSD) model

- **leptodermous expansion--curvature terms**

$$\begin{aligned} E_{mac} &= b_{surf}(1-\kappa_{surf}I^2)A^{2/3}B_{surf}(def) \\ &+ b_{cur}(1-\kappa_{cur}I^2)A^{1/3}B_{cur}(def) \\ &+ \frac{3}{5}\frac{e^2}{4\pi\varepsilon_0}\frac{Z^2}{r_0A^{1/3}}B_{Coul} \end{aligned}$$

The corresponding parameters of … are adjusted to the … nuclear binding energies, **2766** binding energies of nuclei with Z>8 and N>8, … **rms deviation 0.698 MeV**.

K. Pomorski and J. Dudek, Phys. Rev. C **67**, 044316 (2003).

5D PES calculation

Microscopic energy—Strutinsky correction

- **folded-Yukawa potential**

$$\hat{H}=\frac{\mathbf{p}^2}{2M}+\hat{V}_1+\hat{V_{SO}}+\hat{V}_c$$

$$V_1(\mathbf{r})=-\frac{V_0}{4\pi a^3}\int_V\frac{e^{-|\mathbf{r}-\mathbf{r}'|/a}}{|\mathbf{r}-\mathbf{r}'|/a}d\mathbf{r}'$$

$$V_{SO}=-\frac{\lambda}{2M^2c^2}\mathbf{s}\cdot[\nabla V_1\times\mathbf{p}]$$

- **double-center oscillator bases**
- **SBCS**

M. Bolsterli, E. O. Fiset, J. R. Nix, and J. L. Norton, Phys. Rev. C **5**, 1050 (1972).
H. Olofsson, R. Bengtsson, and P. Möller, Nucl. Phys. A **784**, 104 (2007).
J. Maruhn and W. Greiner, Zeitschrift F\“{u}r Phys. **251**, 431 (1972).

5D PES calculation

$$\left[\frac{\mathbf{p}^2}{2m}+\frac{m\omega_\rho^2}{2}\rho^2+\frac{m\omega_{z_{1,2}}^2}{2}\left(z-z_{1,2}\right)^2\right]\Psi=\mathrm{E}\Psi$$

[redacted]

- **The double-center oscillator parameters** $\left(\omega_\rho=?\ \&\ \omega_z=?\right)$
- **Values of quantum number in ζ direction ($n_{\zeta_i}=?$)—not integer**
- **Normalization parameters C_1 and C_2**

→ **Double center oscillator bases**

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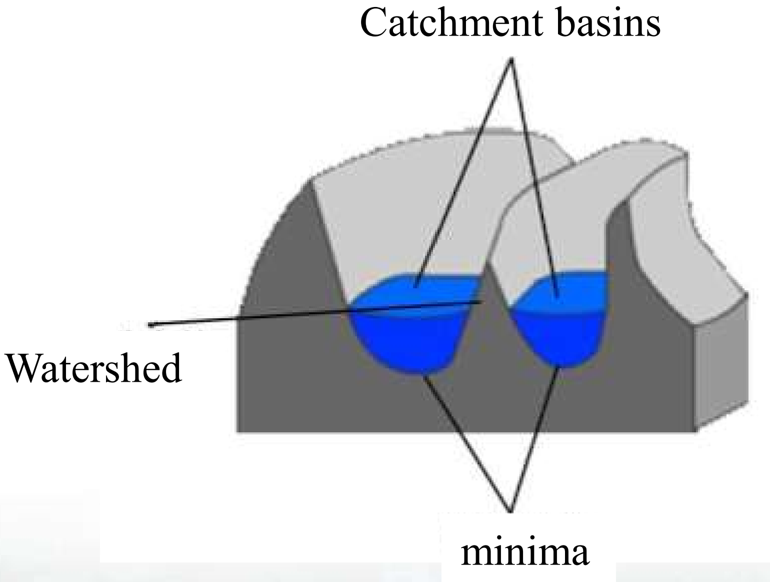
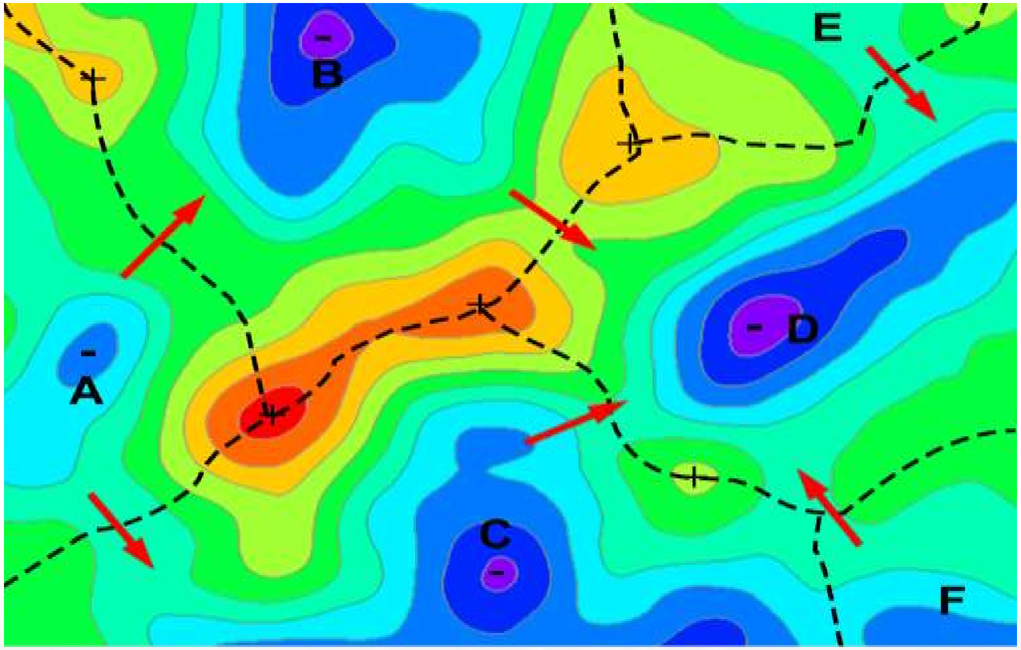
Height of Fission Barriers—Search Algorithm

Rain falling watershed algorithm

Hypothesis: ‘Water’ is supposed to follow the gradient descent path or optimal fission path. If a heavy rain pours over the entire investigated region the optimal path between two arbitrary minima can be found through tracking the surface runoffs.





ZHONG Chun-Lai, et al. Commun. Theor. Phys. 62 (2014) 405–409
L. Vincent et al., IEEE Transactions on Pattern Analysis and Machine Intelligence, 13 (1991) 583
P. D. Smet, et al. Proc. of SPIE’00. San Diego, CA, USA: [s. n.], 2000: 759-766

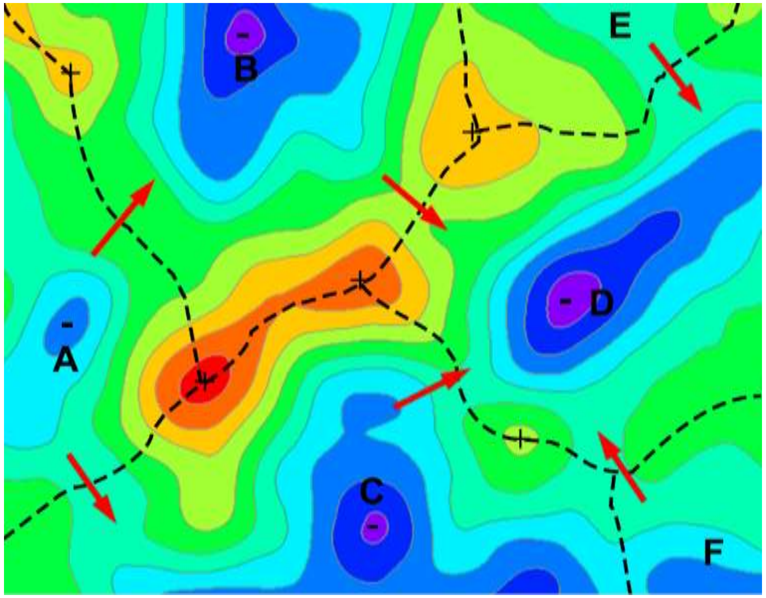
Height of Fission Barriers—Search Algorithm

Scan all the grid points to find local minimums

Scan all the grid points to divide the landscape into basins by minima

Scan all the grid points to identify “watershed”

Search saddle points and fission channels



ZHONG Chun-Lai, et al. Commun. Theor. Phys. 62 (2014) 405–409
L. Vincent et al., IEEE Transactions on Pattern Analysis and Machine Intelligence, 13 (1991) 583
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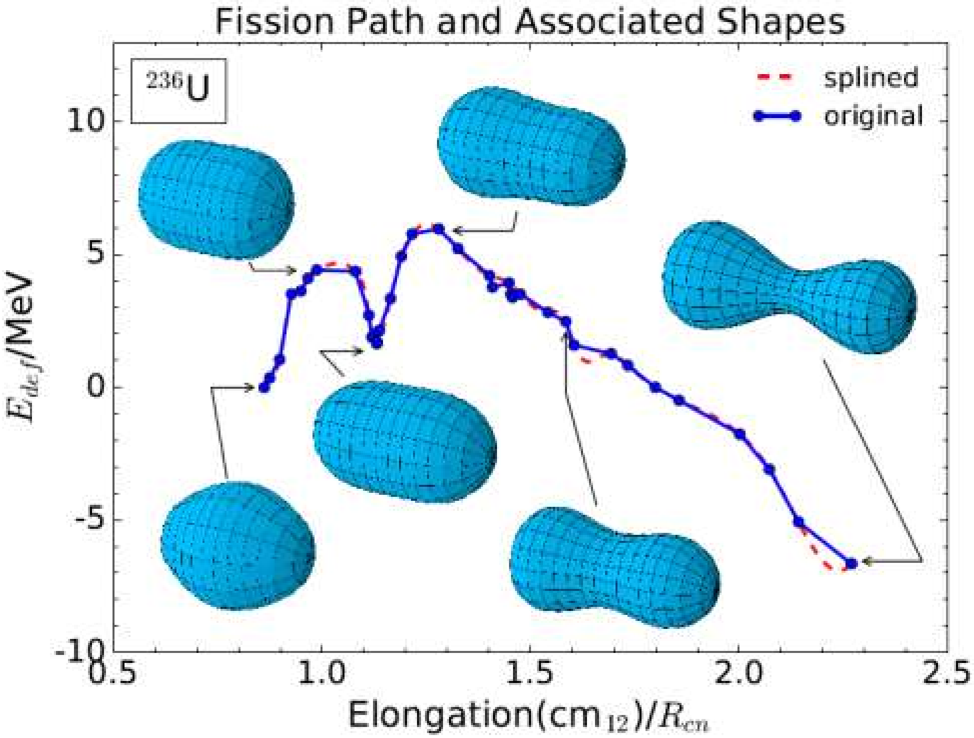
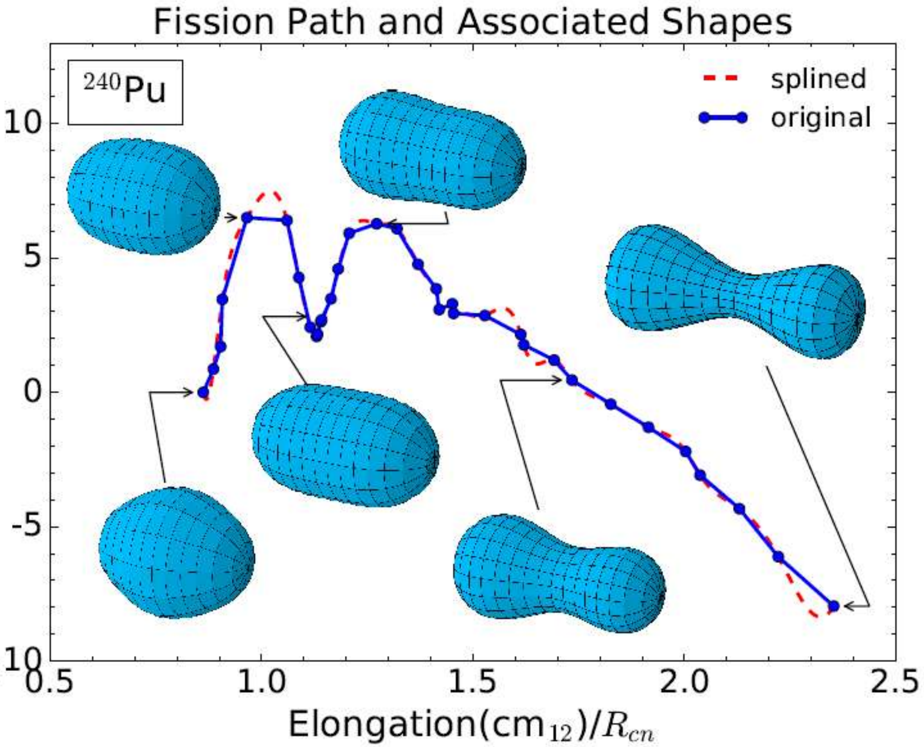
Height of Fission Barriers

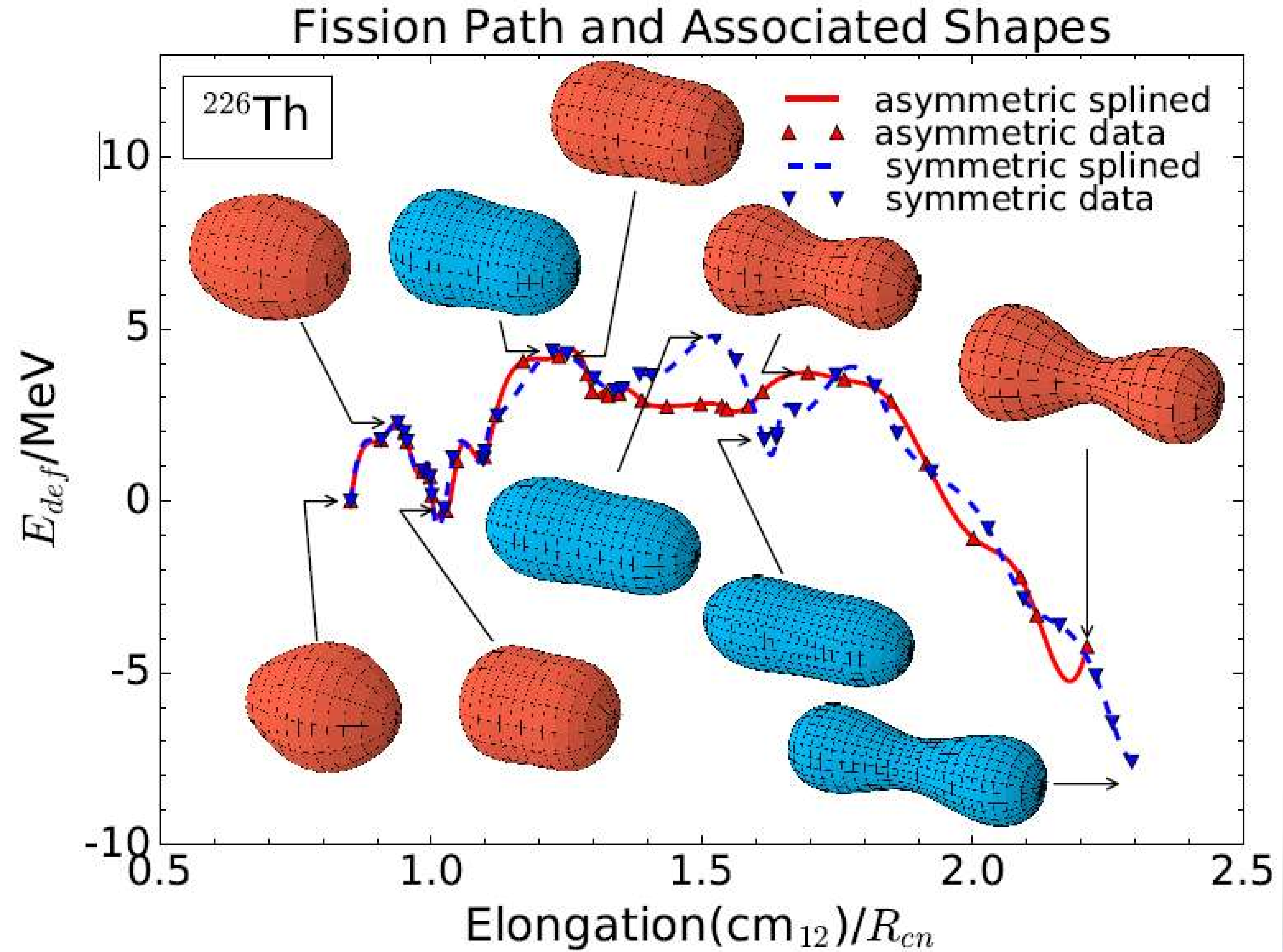


^{236}U fission path



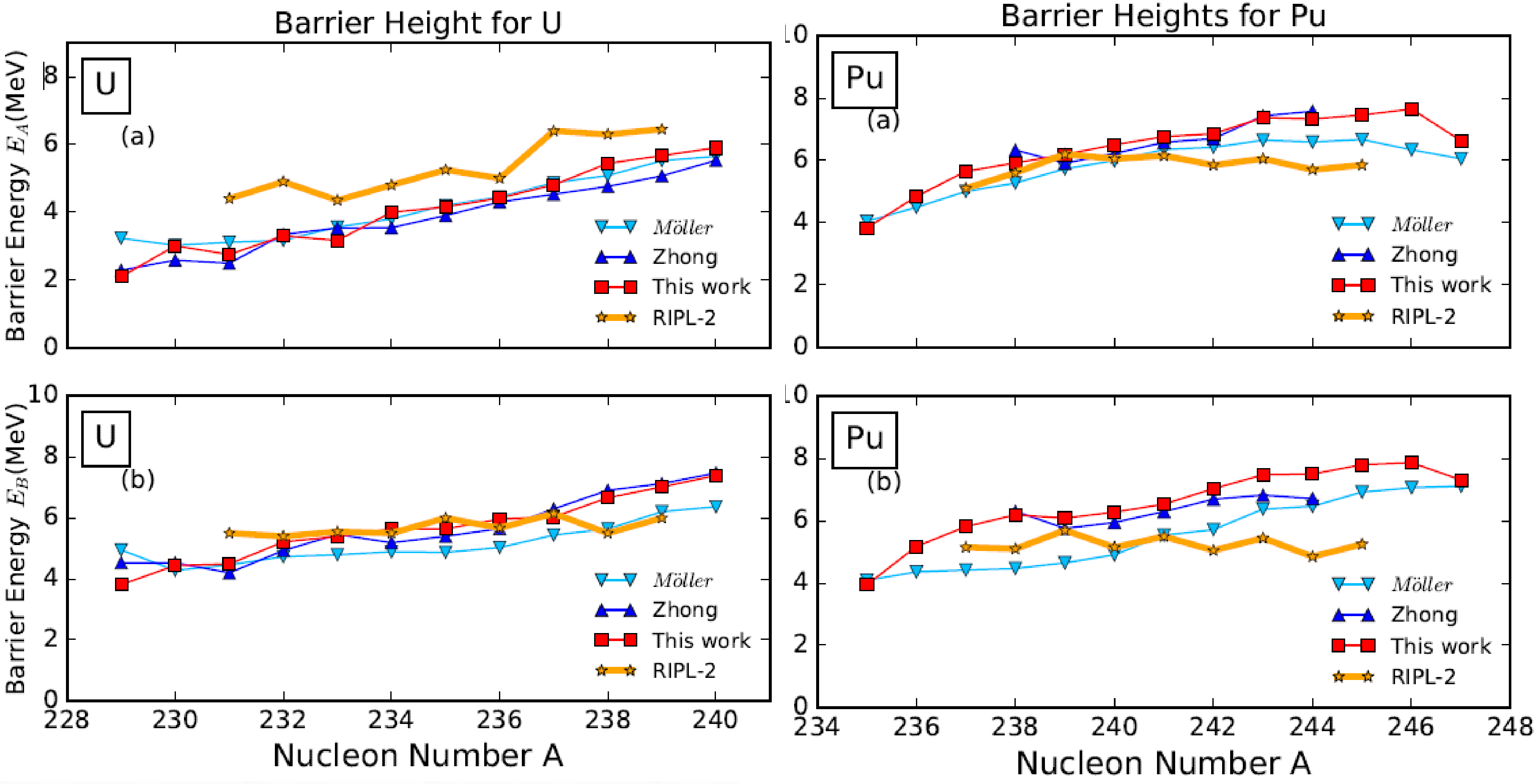
^{240}Pu fission path

Height of Fission Barriers



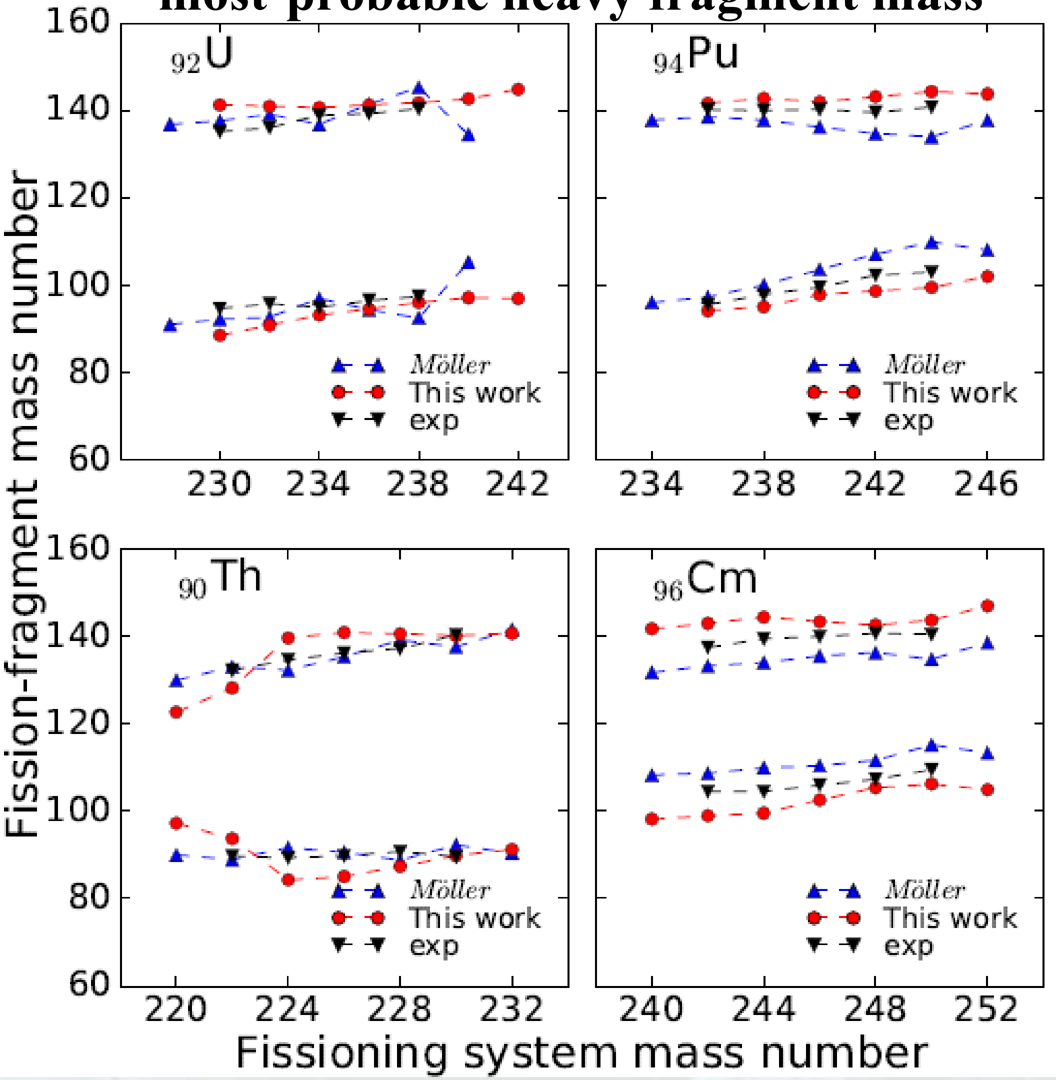
^{226}Th fission path

Height of Fission Barriers



FFMD—Static Analysis

most-probable heavy fragment mass



P. Möller, D. G. Madland, a J. Sierk, and A. Iwamoto, Nature ***409****, 785 (2001).*

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Summary

- **Establish a new MM model and calculate 10 million grids on the five dimensional PESs of several actinide isotopes**

	Shape description	**Macroscopic energy**	**Microscopic energy**	
Möller et al.	Three quadrature surface	FRLDM	Folded-Yukawa	Single center bases
Chiba et al.	Double center oscillator contour	FRLDM	Double center oscillator or Woods-Saxon	Double center bases
This work	**GLS**	**LSD**	**Folded-Yukawa**	**Double center bases**

Summary

- **A new algorithm to find the optimal path and fission barriers. For the scission criterion, we choose the Rayleigh criterion for the point whereby the nucleus splits into fragments**

- **Fission barriers and most-probable heavy fragment masses obtained. Our results shows a consistency with both experimental results and the systematic works of Möller's**