## Multidimensional random walk for calculating the fusion/fission probabilities of superheavy elements

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25.04.2024

Seminarium Fizyki Jądra Atomowego

## Superheavy elements

- Only man-made
- Z>103 (transactinides)
- Produced in nuclear reactions:
- Cold fusion
- Hot fusion


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## Superheavy elements

Oganessian, Yu. (2006). Synthesis and decay properties of superheavy elements. Pure and Applied Chemistry - PURE APPL CHEM. 78. 889-904. 10.1351/pac200678050889.

- Only man-made
- Z>103 (transactinides)
- Produced in nuclear reactions:
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- Hot fusion



## Cold and hot fusion

- $\mathrm{E}^{*} \approx 30-40 \mathrm{MeV}$
- $\mathrm{E}^{*} \approx 10-20 \mathrm{MeV}$
- Compound system is only weakly heated and is cooled down via emission of just one or two neutrons
- Magic nuclei as targets (spherical shapes)


Sigurd Hofmann, Sergey N. Dmitriev, Claes Fahlander, Jacklyn M. Gates, James B. Roberto and Hideyuki Sakai Report of the 2017 Joint Working Group of IUPAC and IUPAP, Pure Appl. Chem. 2020; 92(9): 1387-1446

- Compound nucleus is quite excited (most often emits 3 neutrons)
- Well-deformed radioactive actinides (Act.) targets
- Doubly magic projectile ${ }^{48} \mathrm{Ca}$ short-lived to be used as targets
- Attempts of going beyond the reactions Act. $+{ }^{48} \mathrm{Ca}$ by using heavier projectiles (like ${ }^{50} \mathrm{Ti}$, ${ }^{54} \mathrm{Cr}$, $\left.{ }^{58} \mathrm{Fe},{ }^{64} \mathrm{Ni}\right)$ gave no results so far.


## Motivation

- Experimentalists use theory to determine the optimal reactions and bombarding energies
- A way to calculate $\mathrm{P}_{\text {fus }}$ would be very helpful in the search for the new elements 119 and 120
- We wanted to use the micro-macro model with the inclusion of rotational energy and a random walk method on potential energy surfaces (PES) to calculate the probability of fusion, while describing the fusion process
- The model is first tested on cold fusion reactions with near spherical projectiles: ${ }^{48} \mathrm{Ca}+{ }^{208} \mathrm{~Pb},{ }^{50} \mathrm{Ti}+{ }^{208} \mathrm{~Pb}$ and ${ }^{54} \mathrm{Cr}+{ }^{208} \mathrm{~Pb}$


Sigurd Hofmann, Sergey N. Dmitriev, Claes Fahlander, Jacklyn M. Gates, James B. Roberto and Hideyuki Sakai Report of the 2017 Joint Working Group of IUPAC and IUPAP, Pure Appl. Chem. 2020; 92(9): 1387-1446

## Synthesis model



## Capture cross section $\sigma_{\text {cap }}$

- The entrance channel barrier is described by a distribution that can be approximated by a Gaussian function
- The formula for the capture cross section is derived by folding the Gaussian barrier distribution with the classical expression for the fusion cross section

$$
\begin{aligned}
\sigma_{c a p} & =\pi R^{2} \frac{\omega}{E_{\text {c.m. }} \sqrt{2 \pi}}\left[X \sqrt{\pi}(1+\operatorname{erf}(X))+\exp \left(-X^{2}\right)\right]= \\
& =\pi \lambda^{2}\left(2 l_{\text {max }}+1\right)^{2}, \quad \text { where } X=\frac{E_{c . m .}-B_{0}}{\omega \sqrt{2}}
\end{aligned}
$$

$P_{f u s}$ in experiment


Mechanisms Suppressing Superheavy Element Yields in Cold Fusion Reactions
Banerjee et al., PRL 122, 232503 (2019)

(b)

$P_{f u s}$ in experiment

$P_{f u s}$ can be experimentally estimated:

$$
P_{\text {sym }}=\frac{\text { Fusion-Fission cross section }}{\text { Capture cross section }}
$$

Mechanisms Suppressing Superheavy Element Yields in Cold Fusion Reactions
Banerjee et al., PRL 122, 232503 (2019)


$P_{\text {fus }}$ is calculated by solving 1D Smoluchowski Diffusion Equation

## $P_{f u s}$ in Fusion by Diffusion

1D motion approximation The system must overcome an internal barrier $\boldsymbol{H}$ to fuse.

$L$ is the effective elongation (along the fusion path)

## $\mathrm{t}=0$ <br> E <br>  <br> $$
P_{\text {fus }}(l)=\frac{1}{2}\left(1-\operatorname{erf}\left(\sqrt{\frac{H(l)}{T}}\right)\right) \text { when } L_{\text {inj }} \geq L_{\text {saddle }}
$$

$H(l)$ - the function of angular momentum and bombarding energy
$\boldsymbol{T}$ - the temperature depends on available energy




Higer partial waves $l$

$$
=
$$

Higher rotational energy
=
Higher barrier $H(l)$
=
Lower Pfus(l)

## Fusion probability from FbD model

- Highly effective phenomenological approach
- Only takes into account the macroscopic energy
- Limited to 1 shape dimension

T. Cap, M. Kowal, and K. Siwek-Wilczyńska, Phys. Rev. C 105, L051601 (2022)


## Features of the new model

- Using multidimensional deformation space, including the dipole
- Adopting an auxiliary reference frame giving access to otherwise unattainable shapes, specifically the starting configuration
- Adding the shell effect and rotational energy energy to the whole deformation space
- Replacing the Smoluchowski diffusion equation with a biased, unconstrained random walk


## Goals of the new model

- Comparison with fragment mass distributions (fission, fusion-fission, quasi-fission) and TKE (total kinetic energy) distributions from experiments
- Study of the competition between fusion-fission and quasi-fission
- Study of the shape evolution during fusion and fission
- Modeling the effect of angular momentum on fusion, fission and quasi-fission
- Prediction of fusion probabilities for new SHE synthesis reactions


## Binding/Potential energy in SHE

- Macroscopic (liquid drop) and microscopic (shell effects) energy
- Shell effects responsible for superdeformed minimum in actinides
- SHE exist thanks to the shell effects creating the ground state (often deformed)
- The model needs to account for both energies




Properties of heaviest nuclei with $98 \leq Z \leq 126$ and $134 \leq N \leq 192$
P. Jachimowicz ${ }^{\text {a }}$, M. Kowal ${ }^{\text {b,* }}$, J. Skalski ${ }^{\text {b }}$

${ }^{1}$ Institute of Physics, University of Zielona Góra, Szafrana 4a, 65-516 Zielona Góra, Poland
${ }^{b}$ National Centre for Nuclear Research, Pasteura 7, 02-093 Warsaw, Poland
Ground-state and saddle-point shapes and masses for 1305 heavy and superheavy nuclei including odd-A and odd-odd systems. Static fission barrier heights, one- and two-nucleon separation energies, and $Q \alpha$ values.

Microscopic-macroscopic method with the deformed Woods-Saxon single-particle potential and the Yukawa-plus-exponential macroscopic energy taken as the smooth part.

Ground-state shapes and energies are found by the minimization over seven axially-symmetric deformations. A search for saddle-points was performed by using the "imaginary water flow" method in three consecutive stages, using five- (for nonaxial shapes) and seven-dimensional (for reflection-asymmetric shapes) deformation spaces.

Good agreement with the experimental data for actinides.

5

## Warsaw macro-micro model



- Allows to obtain the binding energy for a given nuclear shape $\beta$
- Macroscopic energy normalized with respect to the sphere:

$$
E_{\text {mac }}=E_{\text {mac }}(\text { deformation })-E_{\text {mac }}(\text { sphere })
$$

## Shape parametrization

- An expansion of the nuclear radius $R(\theta, \phi)$ onto spherical harmonics $Y_{\lambda \mu}(\theta, \phi)$ is used:

$$
R(\vartheta, \varphi)=c R_{0}\left\{1+\sum_{\lambda=1}^{\infty} \beta_{\lambda 0} Y_{\lambda 0}(\vartheta, \varphi)\right\}
$$

- For now, shapes in calculations are limited to axially symmetrical ( $\mu=0$ )


2nd minimum


Fission saddle point

Scission point symmetrical fission

## Deformation parameters

- $\beta_{10}$ - dipole, used as an actual shape parameter
- $\beta_{20}$ - quadrupole/elongation
- $\beta_{30}$ - octupole/asymmetry
- $\beta_{40}$-hexadecople/neck parameter

P. Jachimowicz, M. Kowal, and J. Skalski,

Phys. Rev. C 87, 044308 (2013)

## ※틀



## Potential energy surfaces

- Calculating the energy for a wide array of shapes gives multidimensional potential energy surfaces
- Can be minimized in energy and shown as 3 dimensional maps



## Rotational energy $E_{\text {rot }}$

- Rigid body approximation
- Moment of inertia calculated analytically

M. Brack, T. Ledergerber, H. Pauli, A. Jensen, Nuclear Physics A 234, 185-215 (1974)

$$
\begin{aligned}
I_{\perp} & =\frac{1}{5} \rho R_{0}^{5} \int \sin (\theta)\left(\pi \sin ^{2}(\theta)+2 \pi \cos ^{2}(\theta)\right)\left(1+\frac{1}{2} \sqrt{\frac{3}{\pi}} \beta_{10} \cos (\theta)+\frac{1}{4} \sqrt{\frac{5}{\pi}} \beta_{20}\left(3 \cos ^{2}(\theta)-1\right)\right. \\
& \left.+\frac{1}{4} \sqrt{\frac{7}{\pi}} \beta_{30}\left(5 \cos ^{3}(\theta)-3 \cos (\theta)\right)+\frac{1}{16} \sqrt{\frac{9}{\pi}} \beta_{40}\left(35 \cos ^{4}(\theta)-30 \cos ^{2}(\theta)+3\right)\right)^{5} d \theta
\end{aligned}
$$

## Potential energy surfaces with $E_{\text {rot }}$



## Starting point parametrization


T. Cap, A. Augustyn, M. Kowal, K. Siwek-Wilczyńska, "Dipole-Driven Multidimensional Fusion: An Insightful Approach to the Formation of Superheavy Nuclei", submitted to Phys. Rev. C

## What do we have?

- We have a parametrization to describe many nuclear shapes
- We can calculate the macroscopic, microscopic and rotational energy for those shapes, giving us PESs for different I values
- We can determine the starting configuration of the fusion process

Now all we need is a way to move on the PESs from one shape to another
${ }^{48} \mathrm{Ca}+{ }^{208} \mathrm{~Pb}$ $I=0$ asymmetry


## Biased, unconstrained random walk method

- The probability of transitioning from one shape to another is determined by the number of available energy levels for a given shape $\beta->$ biased
$N_{i}\left(\beta_{i}, \ell\right) \propto \exp \left(2 \sqrt{a\left(E_{\text {max }}^{*}\left(\beta_{i}\right)-E_{\text {rot }}\left(\beta_{i}, \ell\right)\right)}\right) \mathrm{a}$ - constant density parameter
- Only one $\beta$ parameter changes at a time, by a step of 0.05 , giving 8 possible directions of movement



$$
P_{i \rightarrow j}(\ell)=\frac{N_{j}\left(\beta_{j}, \ell\right)}{\sum_{k=1}^{8} N_{k}\left(\beta_{k}, \ell\right)}
$$

## Biased, unconstrained random walk method

- The random walk occurs in a space where the dimensions $\beta_{20}, \beta_{30}$, and $\beta_{40}$ are unconstrained, while $\left|\beta_{10}\right|<1.6$.
- The random walk process continues until an end condition is met, either fusion or fission.
- Fusion is reached after crossing the saddle point ( $\beta_{20} \leq 0.3,\left|\beta_{30}\right| \leq 0.2$, and $\left|\beta_{40}\right| \leq 0.2$ ). Splitting occurs when the neck thickness is less than 3 fm .
- Reaching the end condition for a specific collision energy and angular momentum value defines a single path.



## Example of a paths <br> ${ }^{54} \mathrm{Cr}+{ }^{208} \mathrm{~Pb}$ <br> $E^{*}=50 \mathrm{MeV}, I=40$



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## Biased, unconstrained random walk method

- Calculations were done for excitation energies from 15 to 70 MeV with 1 MeV step. $10^{5}$ paths were calculated for a given energy and $l$-value from 0 to $I_{\text {max }} \cdot \mathrm{P}_{\text {fus }}\left(\mathrm{E}_{\mathrm{cm}}, l\right)$ is given as a ratio of the number of paths that lead to fusion to the total number of paths
$P_{f u s}\left(E_{c m} I\right)=\frac{\text { paths which ended in fusion }}{10^{5}}$
- $\sim 3000 \mathrm{E}^{*}$ and / combinations $\rightarrow \sim 300$ million paths per reaction


## Capture and fusion cross section

- Capture cross section calculated from FbD model
- Fusion cross section from the random walk method $\sigma_{f u s}=\pi \lambda^{2} \sum_{l=0}^{l_{\text {max }}}(2 l+1) T(l) P_{\text {fus }}(l)=\sigma_{c a p} \times P_{\text {fus }}$
- Distributions of $\frac{d \sigma_{c a n}}{d l}$ (black) and $\frac{d \sigma_{\text {fus }}}{d l}$ (red) for ${ }^{48} \mathrm{Ca}+{ }^{208} \mathrm{~Pb}$

$E^{*}=20 \mathrm{MeV}$

$E^{*}=40 \mathrm{MeV}$


$$
\mathrm{E}^{*}=60 \mathrm{MeV}
$$

## Fusion probability from the random walk

Average over / to get $P_{f u s}$ dependant on $\mathrm{E}_{\mathrm{cm}}: P_{f u s}\left(E_{c m}\right)=\frac{\sum_{l=0}^{\max }(2 l+1) P_{f u s}(l)}{\left(2 l_{\max }+1\right)^{2}}$ fusion probability averaged over $l$


The averaged fusion probabilities < Pfus > (solid black lines) calculated using the random walk method for the
 The arrows represent the locations of the mean entrance channel barrier $B_{0}$ for each reaction.

## Mass distribution of fission fragments

- The final fission shapes can be divided, and their volumes compared, giving the mass distribution of fission fragments, for each $\mathrm{E}^{*}$ and $l$.




## Next steps for fusion

- Expand to $8 \beta_{\lambda 0}$ dimensions
- Determine optimal step size for each $\beta$ parameter
- Expand the model to describe under barrier reactions
- Expand to non-axially symmetric shapes ( $\beta_{\lambda \mu}$ ) and incorporate multiple possible starting points depending on the orientation of the target and the projectile
- Introduce a density parameter beyond Fermi gas model and incorporate shellcorrection damping
- Allow for the emission of neutrons, protons and alfa particles during the random walk


## Emission of neutrons, protons and alfa particles during the random walk

Instead of moving only between shapes, we can also change the PESs.

$$
{ }^{52} \mathrm{Cr}+{ }^{208} \mathrm{~Pb}, \mathrm{I}=0
$$

## Random walk in fission

- Start in the excited ground state/saddle /second minimum
- Continue the random walk until fission
- Could be used in conjunction with the fusion random walk to describe mass fragment distributions from the fusion-fission process
- Could be used to describe mass fragment distributions from neutron induced fission
- Number of steps is multiple orders of magnitude higher than in fusion, increasing the lower the excitation energy



## Summary

- The random walk method reproduces experimental results for probability of fusion, even though there are no fitted parameters within the model itself
- Including the $\beta_{10}$ as an actual shape variable allowed to describe the starting point configuration with only 4 deformation parameters
- The new approach makes possible to predict mass fragment distributions, which can be compared with experimental data
- The random walk method looks to be a promising direction of study, both for fusion and fission of superheavy nuclei


## Thank you for your attention!

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