Time-Dependent Hartree-Fock Approach to SHE Dynamics

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Collaborators:

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Erlangen:	P.-G. Reinhard	**Indiana:**	C. Horowitz
Surrey:	P.D. Stevenson		

Topics:

Time-dependent DFT theory

Fusion, Capture (DC-TDHF)

Quasifission using TDHF, PCN

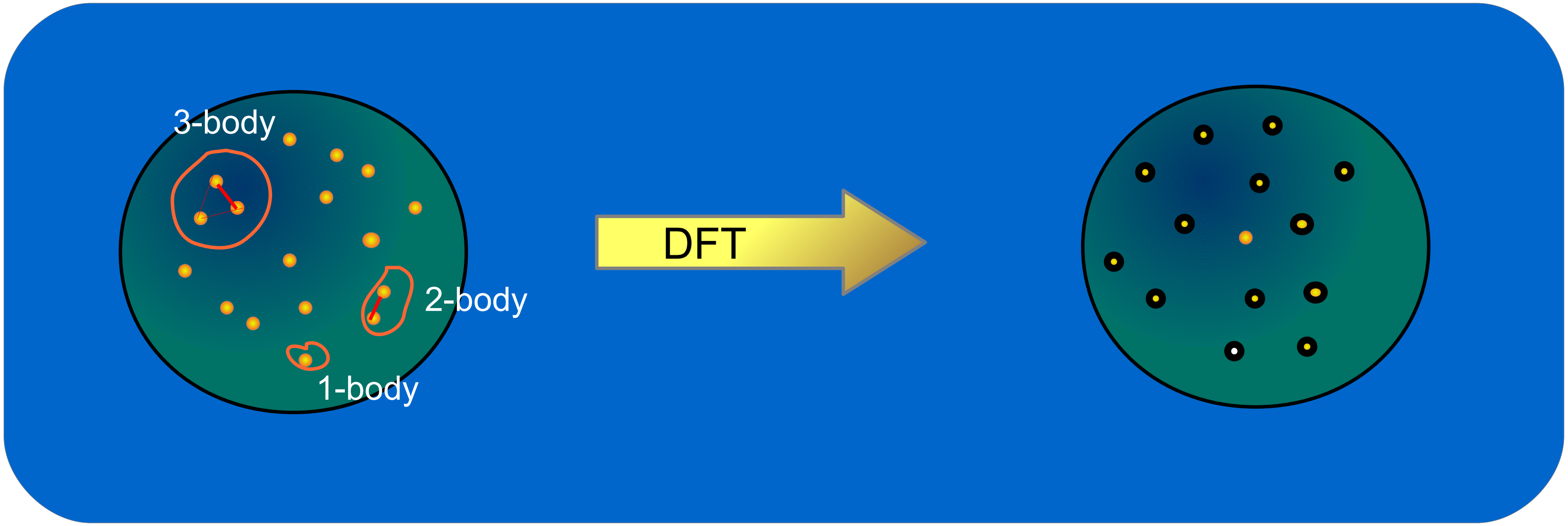
Dynamics of Fission

Deep-inelastic collisions (optional)

Conclusions

Research supported by: U.S. Department of Energy, Division of Nuclear Physics

Nuclear Mean Field or Energy Density Functional (EDF)



ab-initio

$$\langle \Psi | H | \Psi \rangle = E$$

Mean-field - EDF

$$\Psi \to \Phi_{Slater}$$

$$H \to H_{eff}$$

$$E = \langle \Phi | H_{eff} | \Phi \rangle = \int d^3 r \; \{ H(\rho, \tau, \boldsymbol{j}, \boldsymbol{s}, \boldsymbol{T}, J_{\mu\nu} \; ; \boldsymbol{r}) + H_{Coulomb}(\rho_p) \}$$

Single-(one-) particle density *etc.* in terms of s.p. states

$$\rho_q(\boldsymbol{r}) = \sum_{i=1}^{A} \sum_{\sigma} \varphi_i^*(\boldsymbol{r}, \sigma, q) \varphi_i(\boldsymbol{r}, \sigma, q)$$

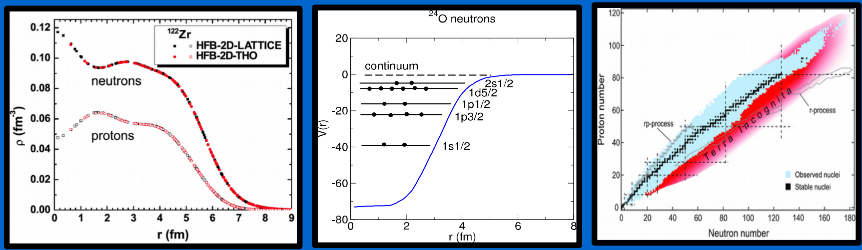
EDF in NP more complicated

$$v = v_{NN-eff} \to DFT\,(Hartee - Fock)$$

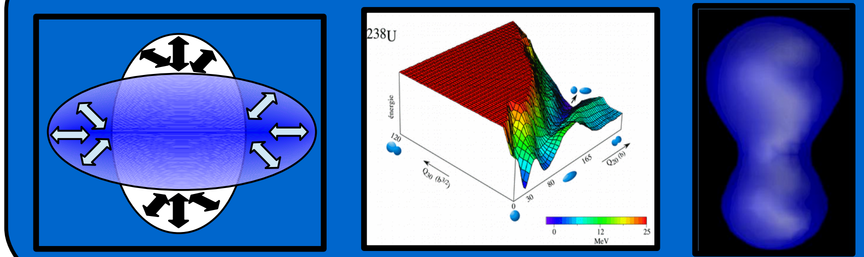
$$v \neq v_{NN-eff} \to DFT\,(Kohn - Sham)$$

Study Structure, Reactions, and Star Matter in Same Framework

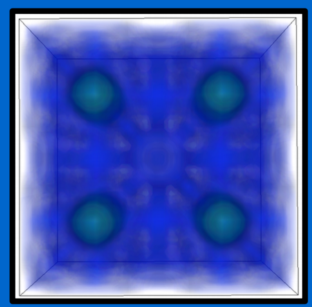
Structure



Oscillations, Fusion, Fission



Neutron Star Crust



- Time-dependent generalization TDHF or TDDFT (variational or Runge-Gross)

$$\delta S=\delta\int_{t_1}^{t_2} dt\,\langle\Phi(t)|H_{eff}-i\hbar\partial_t|\Phi(t)\rangle=0$$

$$i\frac{\partial}{\partial t}\varphi_\alpha=h(\rho,\tau,\boldsymbol{j},\boldsymbol{s},\boldsymbol{T},J_{\mu\nu};\boldsymbol{r})\varphi_\alpha$$

self-consistent

- TDHF gives the *most probable outcome* – best if *x*-section dominated by one process

Nuclear Energy Density Functional

$$
\begin{aligned}
H_S(\boldsymbol{r}) = {} & \frac{\hbar^2}{2\mathrm{m}}\tau+\frac{1}{2}t_0\left(1+\frac{1}{2}x_0\right)\rho^2-\frac{1}{2}t_0\left(\frac{1}{2}+x_0\right)\left[\rho_p^2+\rho_n^2\right]+\frac{1}{4}\left[t_1\left(1+\frac{1}{2}x_1\right)+t_2\left(1+\frac{1}{2}x_2\right)\right](\rho\tau-\boldsymbol{j}^2) \\
& -\frac{1}{4}\left[t_1\left(\frac{1}{2}+x_1\right)-t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\tau_p+\rho_n\tau_n-\boldsymbol{j}_p^2-\boldsymbol{j}_n^2\right)-\frac{1}{16}\left[3\mathrm{t}_1\left(1+\frac{1}{2}x_1\right)-t_2\left(1+\frac{1}{2}x_2\right)\right]\rho\nabla^2\rho \\
& +\frac{1}{16}\left[3\mathrm{t}_1\left(\frac{1}{2}+x_1\right)+t_2\left(\frac{1}{2}+x_2\right)\right]\left(\rho_p\nabla^2\rho_p+\rho_n\nabla^2\rho_n\right) \\
& +\frac{1}{12}t_3\left[\rho^{\alpha+2}\left(1+\frac{1}{2}x_3\right)-\rho^{\alpha}\left(\rho_p^2+\rho_n^2\right)\left(x_3+\frac{1}{2}\right)\right] \\
& +\frac{1}{4}t_0x_0\boldsymbol{s}^2-\frac{1}{4}t_0(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2)+\frac{1}{24}\rho^{\alpha}t_3x_3\boldsymbol{s}^2-\frac{1}{24}t_3\rho^{\alpha}(\boldsymbol{s}_n^2+\boldsymbol{s}_p^2) \\
& \cancel{+\frac{1}{32}(t_2+3\mathrm{t}_1)\sum_q \boldsymbol{s}_q\cdot\nabla^2\boldsymbol{s}_q-\frac{1}{32}(t_2x_2-3t_1x_1)\boldsymbol{s}\cdot\nabla^2\boldsymbol{s}} \\
& +\frac{1}{8}(t_1x_1+t_2x_2)(\boldsymbol{s}\cdot\boldsymbol{T}-\boldsymbol{J}_{\mu\nu}^2)+\frac{1}{8}(t_2-t_1)\sum_q(\boldsymbol{s}_q\cdot\boldsymbol{T}_q-\boldsymbol{J}_{q\mu\nu}^2) \\
& -\frac{t_4}{2}\sum_{qq'}(1+\delta_{qq'})\left[\boldsymbol{s}_q\cdot\nabla\times\boldsymbol{j}_{q'}+\rho_q\boldsymbol{\nabla}_{\mu\nu}\cdot\boldsymbol{J}_{\mu\nu}\right]
\end{aligned}
$$

Time-odd terms come in pairs!
Total is TR invariant

"s" in t_0 and t_3

Unstable- not used

"s" in spin-orbit

(s,j,T) time-odd, vanish for static HF calculations of even-even nuclei
non-zero for dynamic calculations, odd mass nuclei, cranking etc.

Validity of TDDFT in Nuclear Reactions – Beyond Mean Field

- All or most of $E_{c.m.}$ can be transformed to internal excitation
- Effective s.p. wavelength should be long compared to nuclear size (no hard coll.)

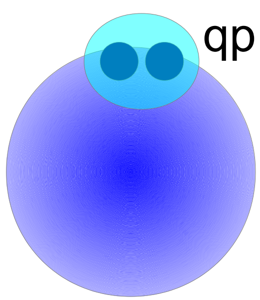
Limits E/A for reactions!

$$\bar{\lambda} \simeq \frac{213.08}{\epsilon^{3/2}} \qquad \epsilon = \frac{(E_{cm} - E_B)}{\mu}$$

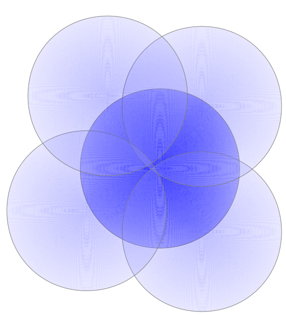
Fermi-Gas
Fermi-Liquid

- Good for inclusive processes with a dominant channel
- Missing many-body correlations limits widths (Balian-Veneroni, projections)

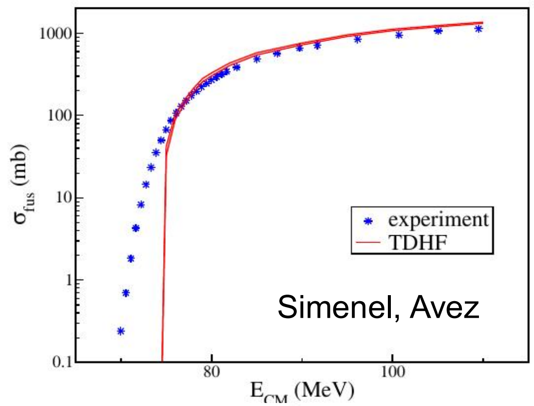
Pairing | Configuration mixing | Subbarrier fusion



Pair transfer, initial structure



Breakup, multiple exit channels



$$\sigma_{fus}(E) = \frac{\pi\hbar^2}{2\mu E}\,[l_{max}(E)+1]^2$$

Anatomy of Low-Energy Heavy-Ion Collisions

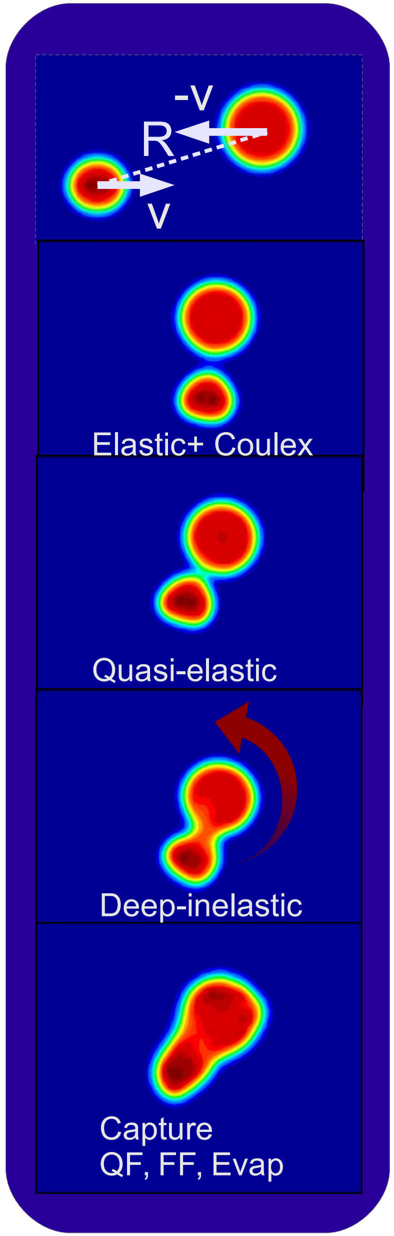
Inelasticity

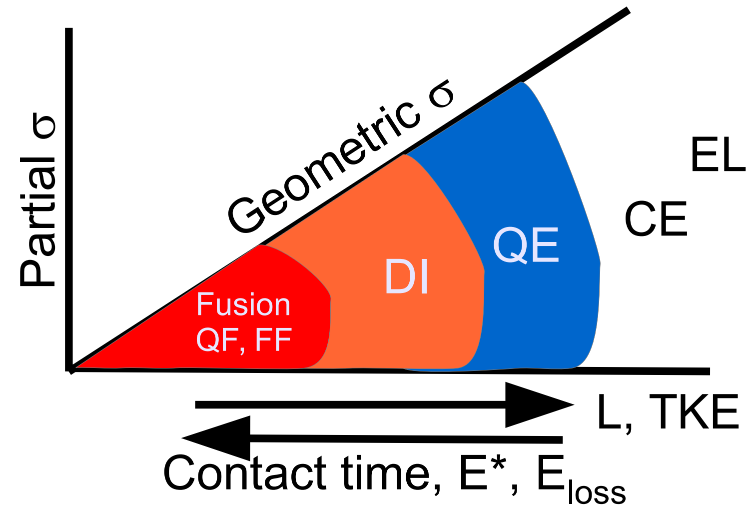
Large b, distant collision
Elastic and Coulomb excitation

Peripheral collision
nucleon+ exchange
Small TKE loss

Deep-inelastic collision
Multi-nucleon exchange
Large TKE loss, L loss

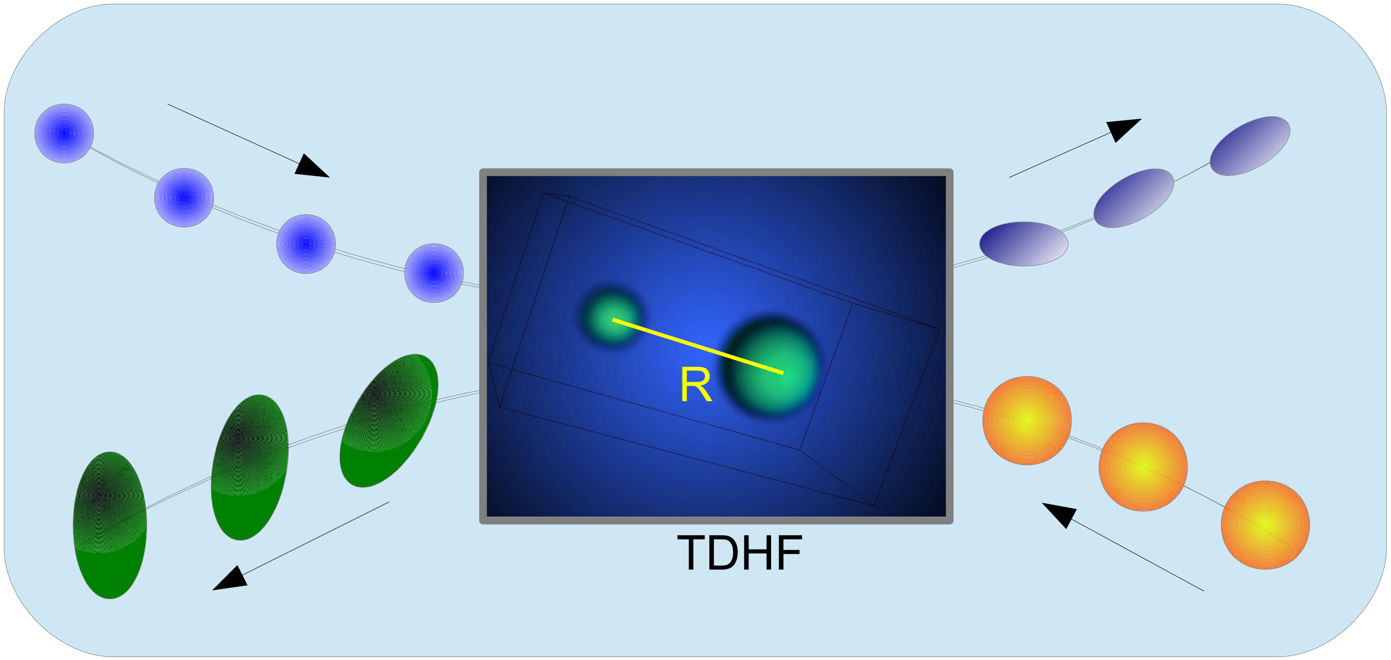
Composite formed
Multi-nucleon exchange
Large TKE loss, L loss
Fusion
Quasi-fission
Fusion-fission
Evaporation residue





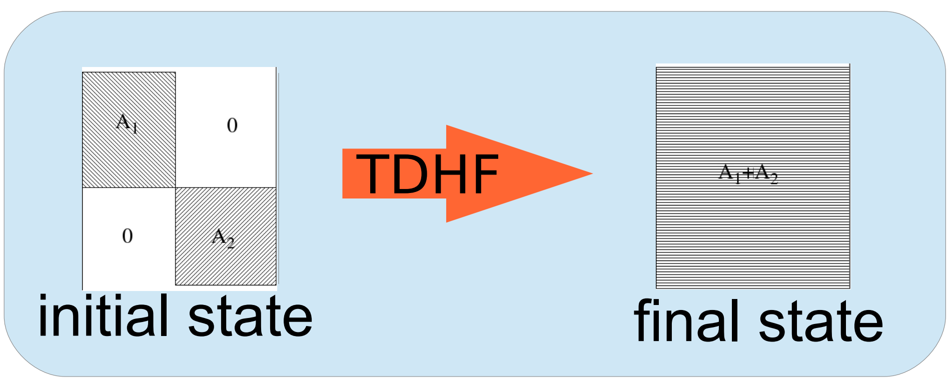
TDHF Initial Setup

- Initial approach is determined by Coulomb trajectory
- The initial DFT Slater determinants boosted by velocities at **R**



If final stage contains a single fragment – FUSION
If final stage contains two fragments – DI, QF

Slater determinant

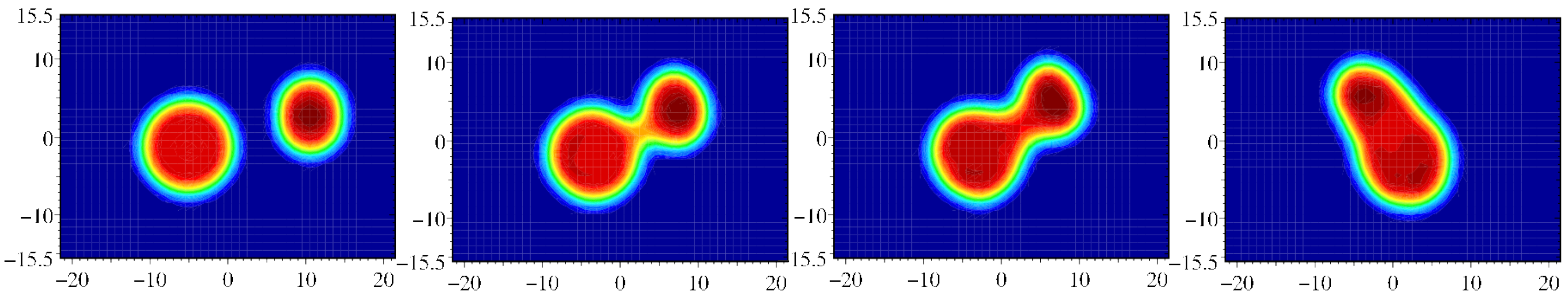


Modern TDHF Codes

<u>VU-TDHF Code</u>

- Basis-Spline discretization for high accuracy
- 3-D Cartesian lattice – no geometrical simplification
- Complete EDF including all terms (time-even, full time-odd)
- Coded in Fortran-95 and OpenMP

1. Umar, Oberacker, VU-TDHF, Phys. Rev. C 73, 054607 (2006)
2. Maruhn, Reinhard, Stevenson, Umar, Sky3D, *Comp. Phys. Comm.* 85, 2195 (2014)



Fusion Phenomenology

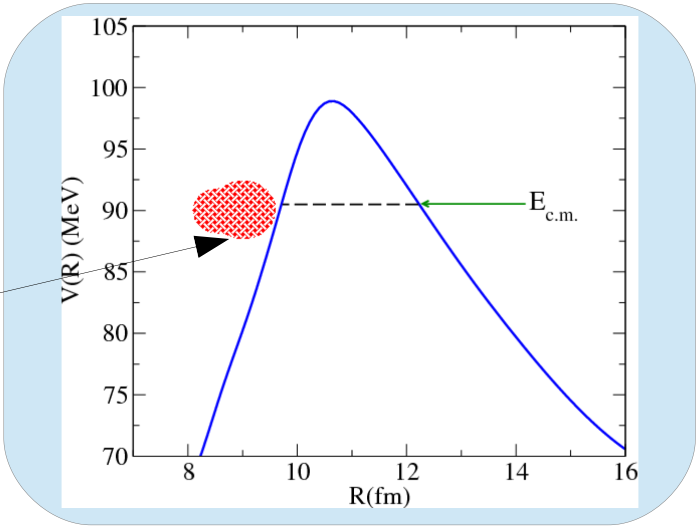
No practical ab-initio many-body theory for dynamical sub-barrier fusion exists. Standard approach involves several steps:

a) Calculate heavy-ion potential V(R)
- phenomenological (Woods-Saxon / proximity potential)
  double-folding model with frozen densities
- macroscopic-microscopic
- two-center shell model + liquid drop
- microscopic: Skyrme + extended Thomas-Fermi

b) Quantum tunneling (either WKB-HW, or solve Schrödinger equation for relative motion R with Incoming Wave Boundary Condition (IWBC))

c) Model inelastic and transfer channels:
- coupled channels approach (Esbensen, Hagino)

Frozen density breaks down
Dynamical rearrangement of density
Excitation of pre-equilibrum states
Dynamical transfer, M(R)



d) Corrections to CC: Compression potential, neck modeling

B. B. Back, H. Esbensen, C. L. Jiang, and K. E. Rehm, Rev. Mod. Phys. 86, 317 (2014)

TDDFT + Density Constraint = Internuclear Potentials

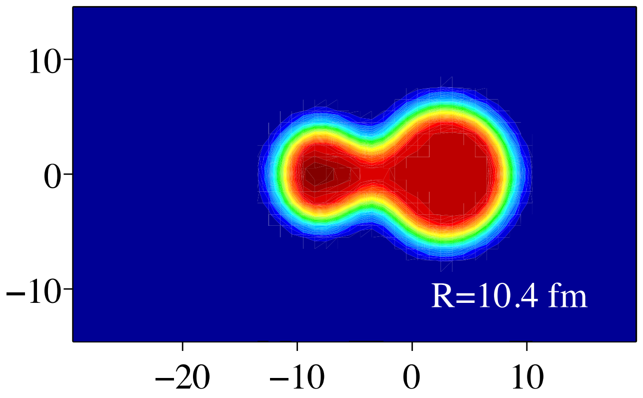
- Minimize energy with density constraint during unhindered TDDFT

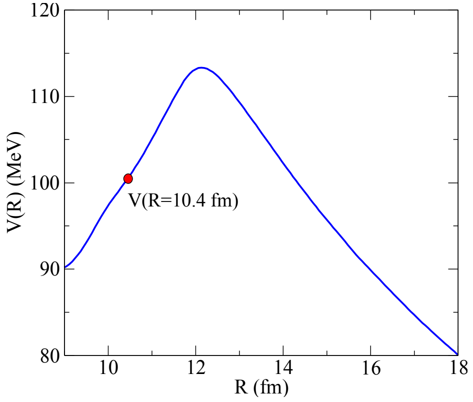
$$E_{DC}(t)=\min_{\rho}\{E[\rho_n,\rho_p]+\int d^3r\, v_n(\boldsymbol{r})[\rho_n(\boldsymbol{r})-\rho_n^{tddft}(\boldsymbol{r},t)]+\int d^3r\, v_p(\boldsymbol{r})[\rho_p(\boldsymbol{r})-\rho_p^{tddft}(\boldsymbol{r},t)]\}$$

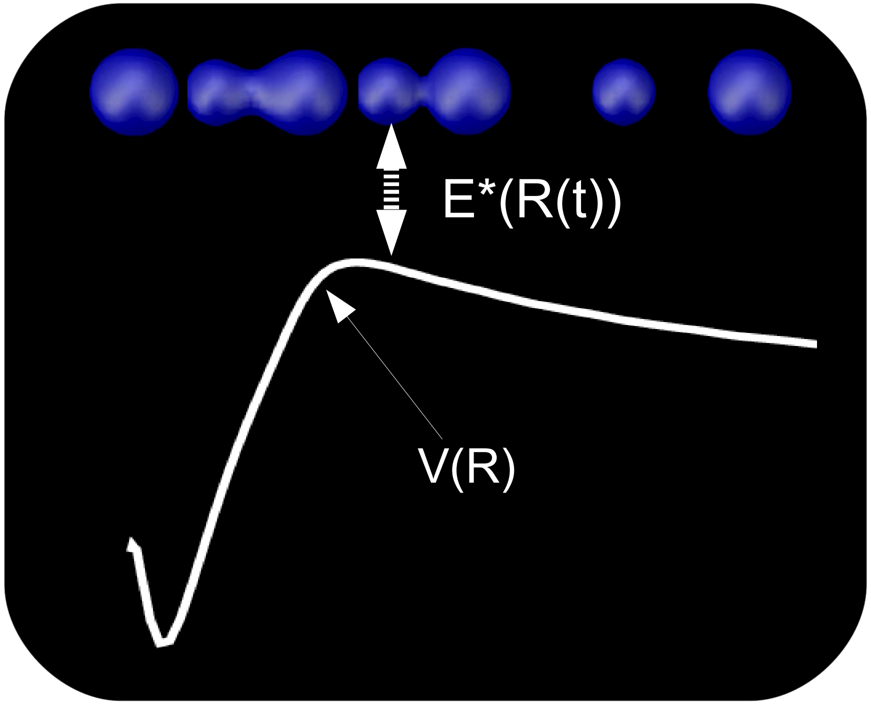
- Goal: find internuclear potential – can calculate subbarrier fusion!

- DC-TDHF finds underlying microscopic potential V(R)
- Parameter-free, only depends on chosen EDF
- Dynamical, energy-dependent
- Calculate E*(t) and M(R)
- Applied to:
  - Fusion of neutron-rich heavy systems
  - Capture for superheavy formations
  - Neutron-rich light systems for astrophysical applications

$$V(R(t))=E_{DC}(t)-E_{A_1}-E_{A_2}$$

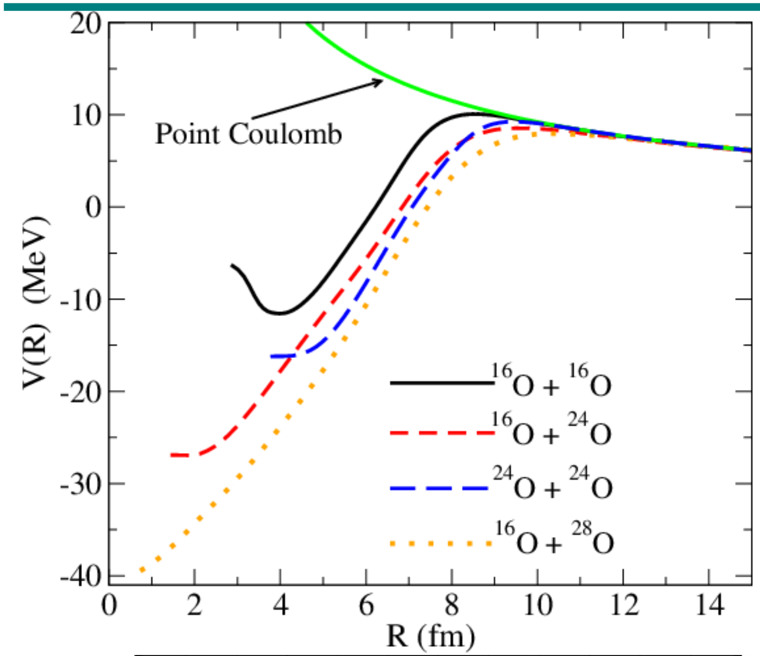


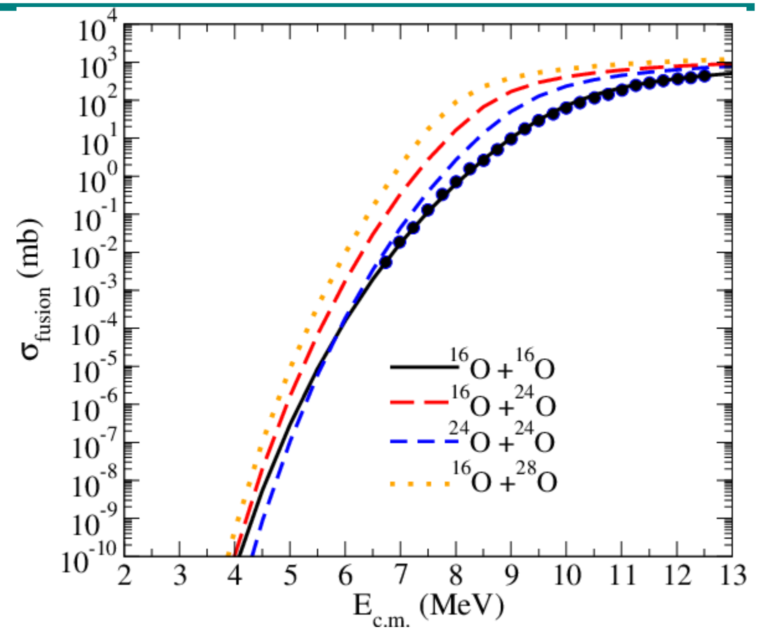


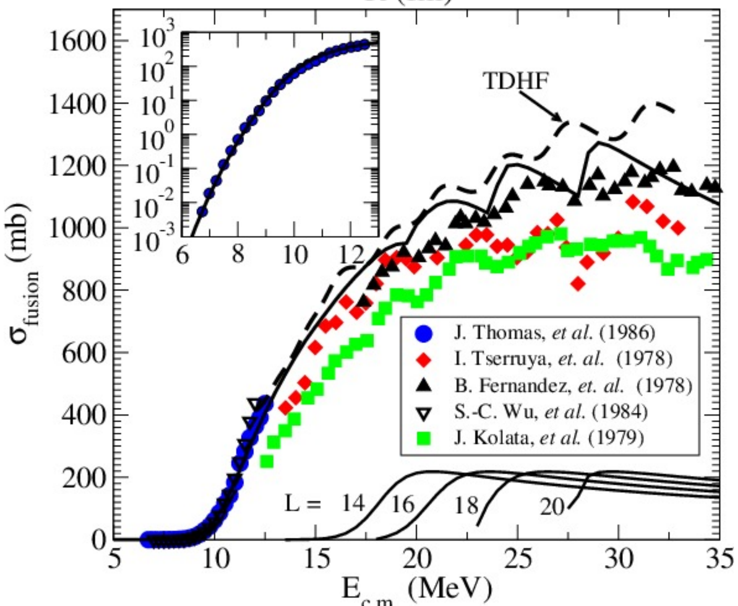


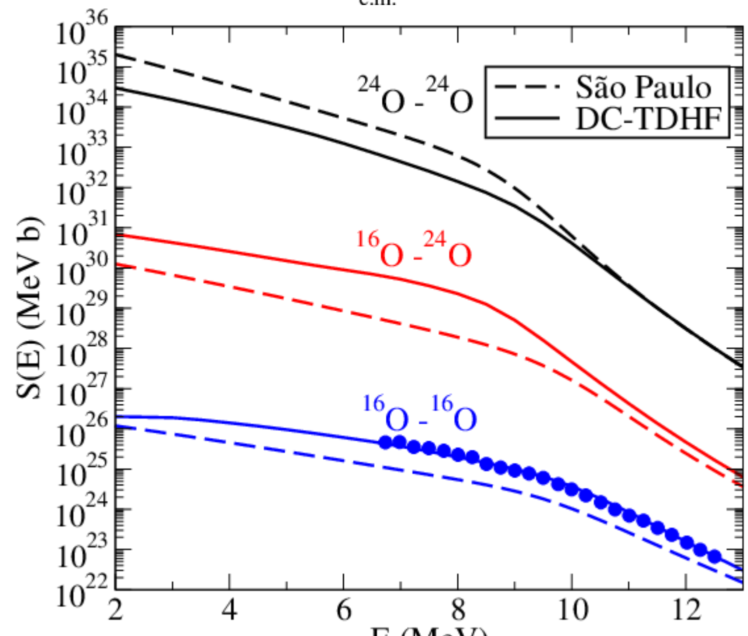
Selected Applications of DC-TDHF
To
Fusion and Capture

Fusion Cross-Sections for $^{16,24}O + ^{16,24,28}O$



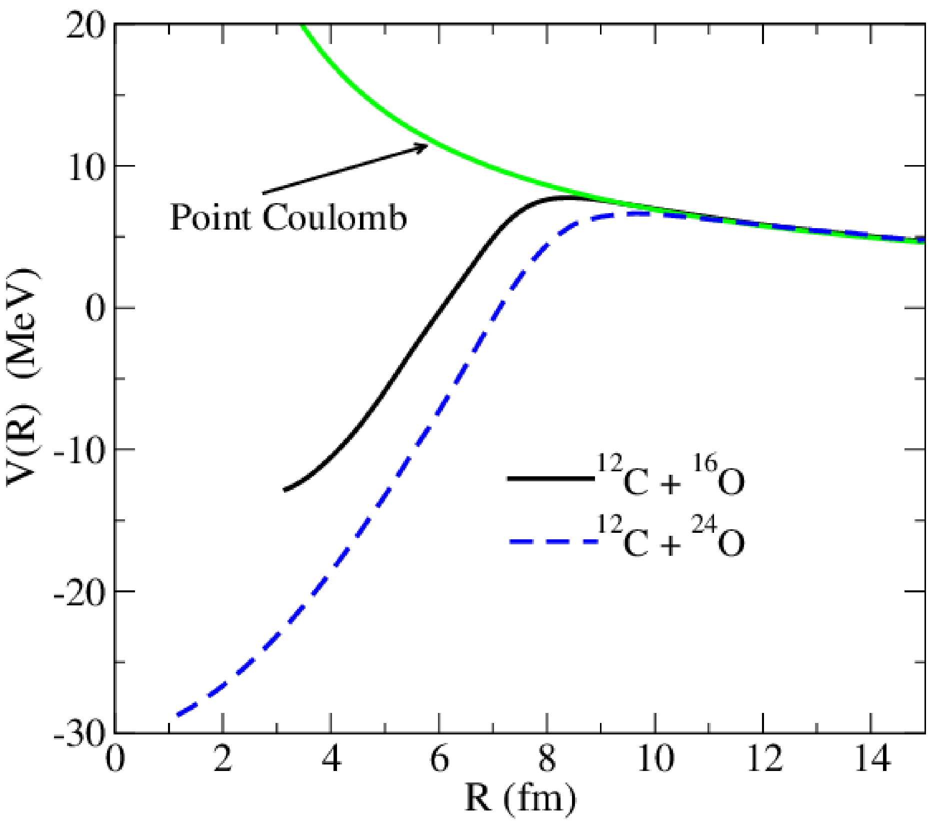


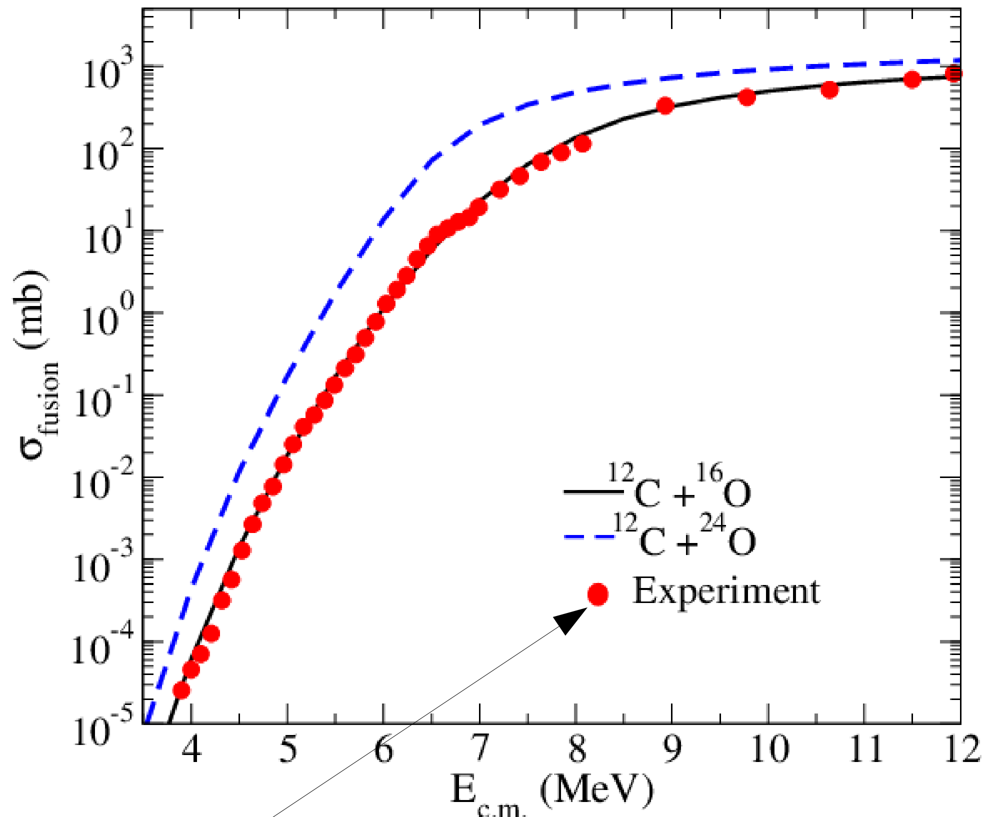




A.S. Umar, V.E. Oberacker, and C. J. Horowitz, PRC **85**, 055801 (2012)
C. Simenel, R. Keser, A.S. Umar, V.E. Oberacker, Phys. Rev. C **88**, 024617 (2013)

Fusion Cross-Sections for $^{12}C+^{16,24}O$



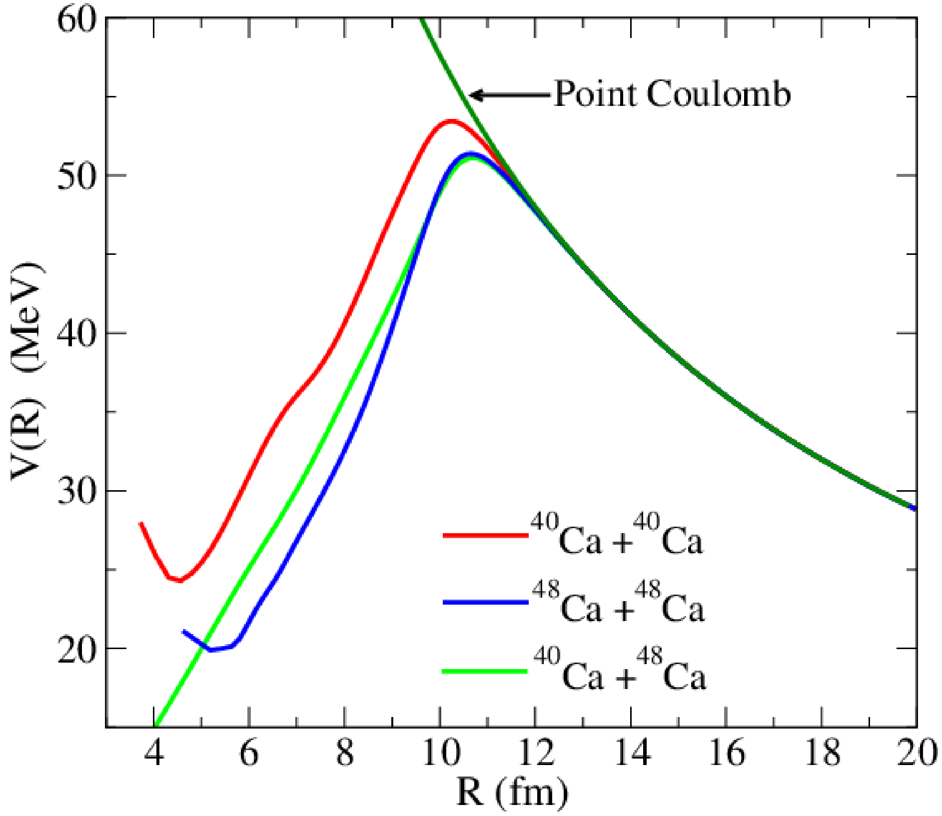


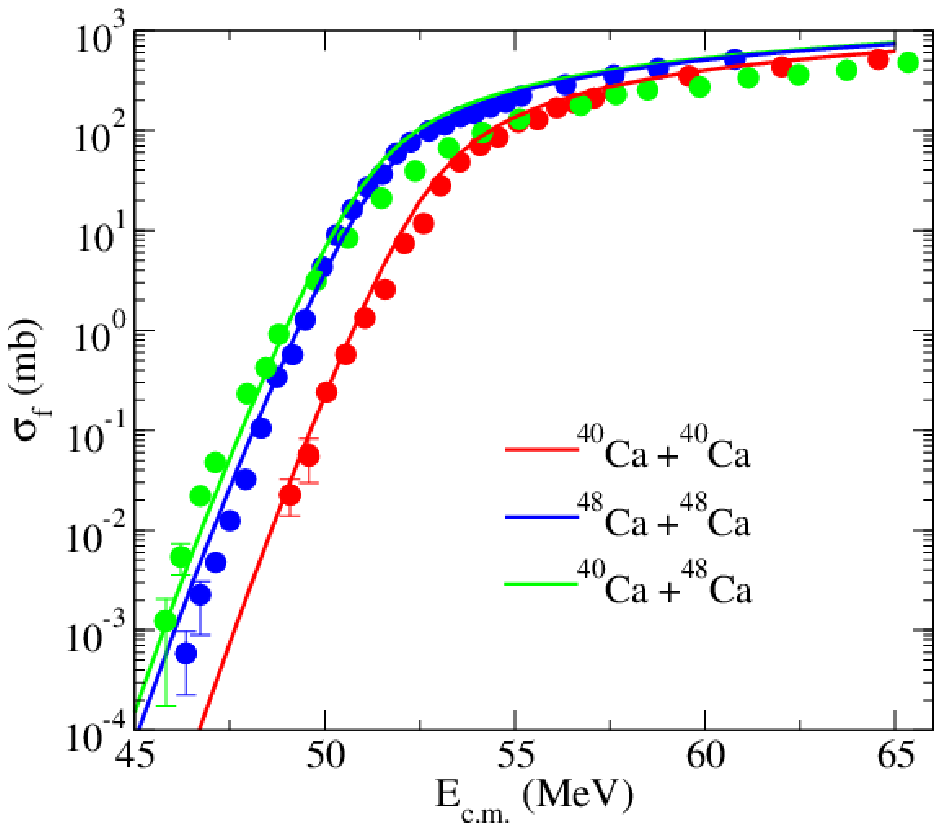
barrier heights (MeV)
7.77
6.64

P. R. Christensen *et al.*, Nucl. Phys. A**280**, 189 (1977)

A.S. Umar, V.E. Oberacker, and C. J. Horowitz, PRC **85**, 055801 (2012)

Fusion for ^{40}Ca + ^{40}Ca, ^{48}Ca + ^{48}Ca, ^{40}Ca + ^{48}Ca



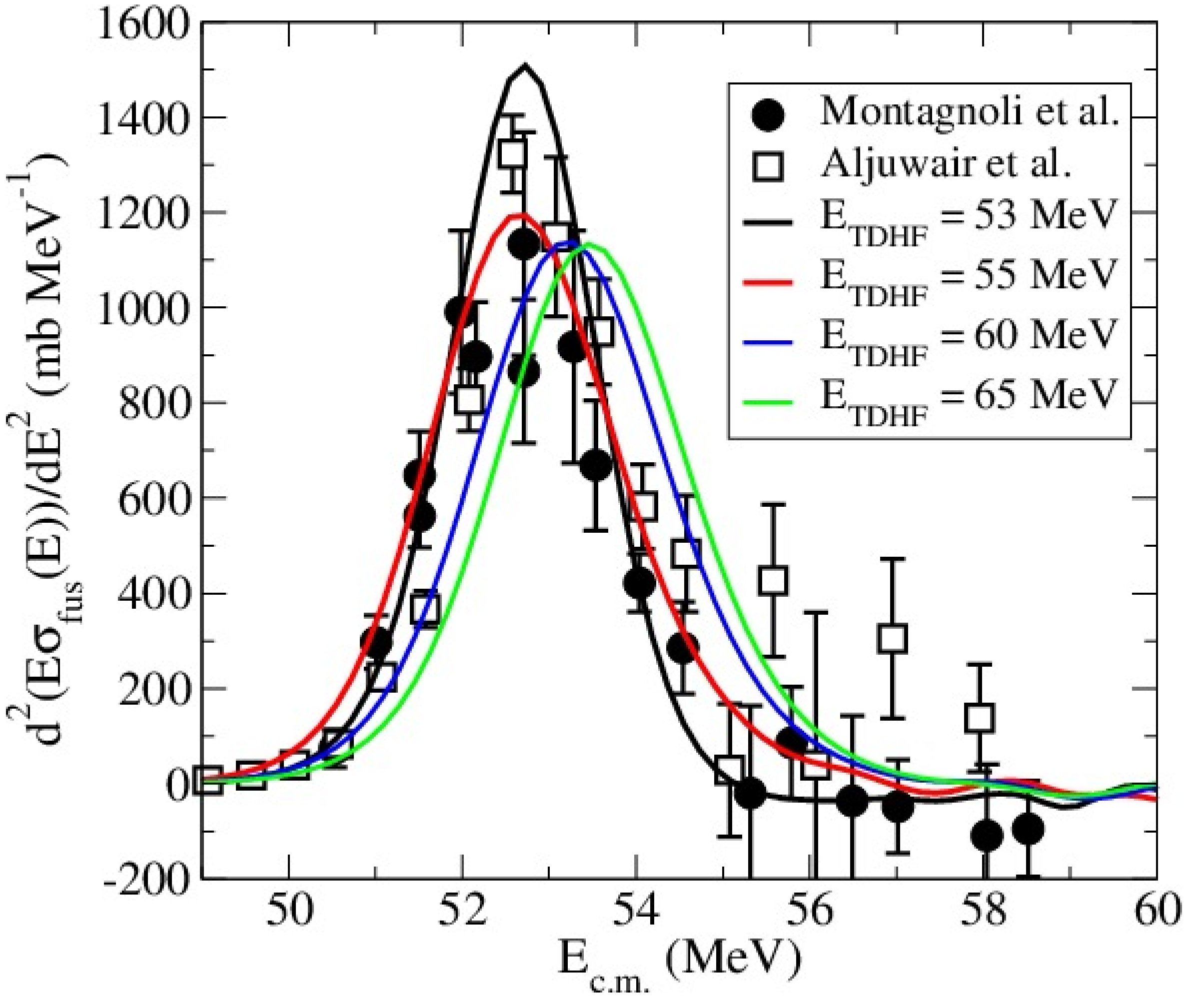


- 40Ca and 48Ca usually in Skyrme fits (here SLy4) but shell structure not that good
- Small deviations due to small c.m. energy dependence of V(R)
- High E part of 40Ca+48Ca and low E part of 48Ca+48Ca show larger deviations

exp. data:
G. Montagnoli *et al.*, PRC **85**, 024607 (2012)
A. M. Stefanini *et al.*, Phys. Lett. B **679**, 95 (2009)
C. L. Jiang *et al.*, PRC **82**, 041601(R) (2010)

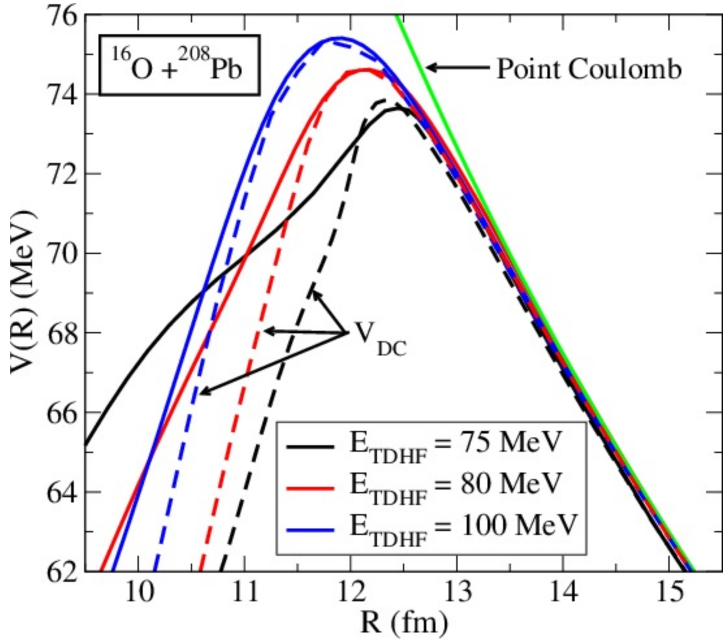
R. Keser, A. S. Umar, and V. E. Oberacker, Phys. Rev. C **85**, 044606 (2012)

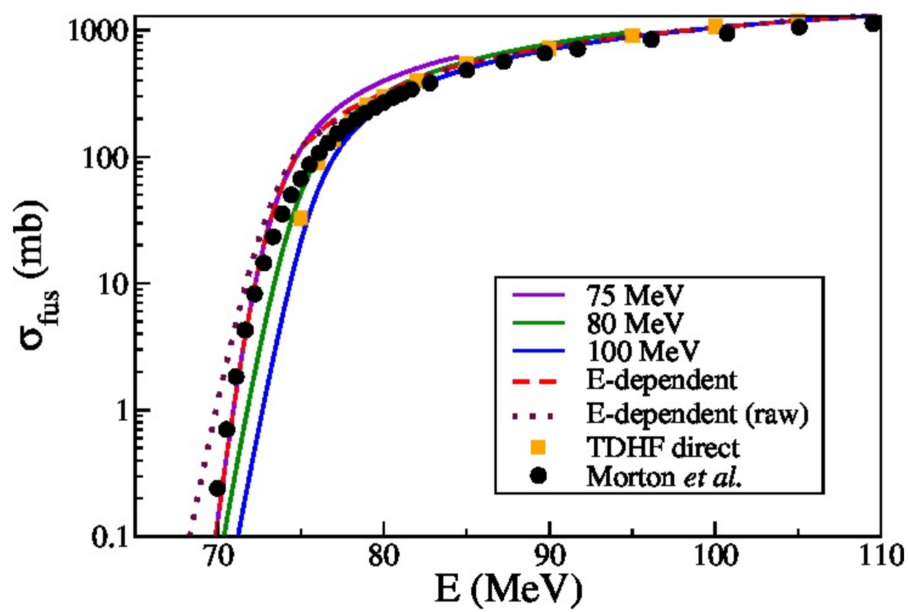
Fusion Barrier Distributions

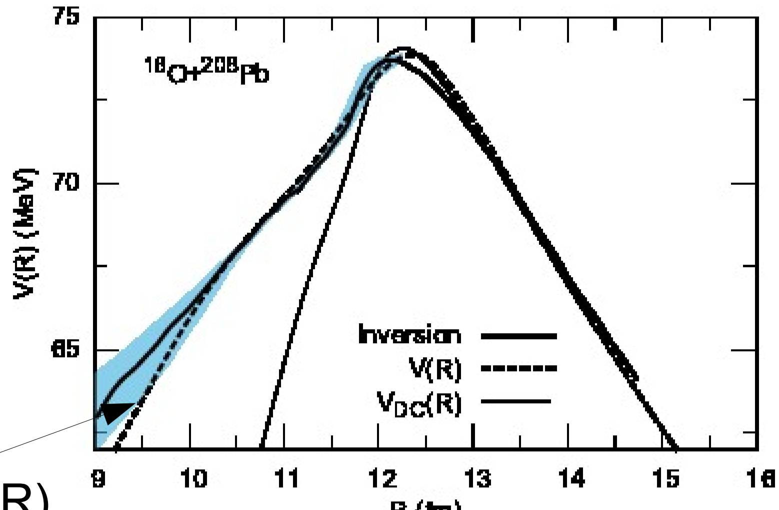


A. S. Umar, C. Simenel, and V. E. Oberacker, Phys. Rev. C **89**, 034611 (2014)

Fusion for $^{16}O + ^{208}Pb$

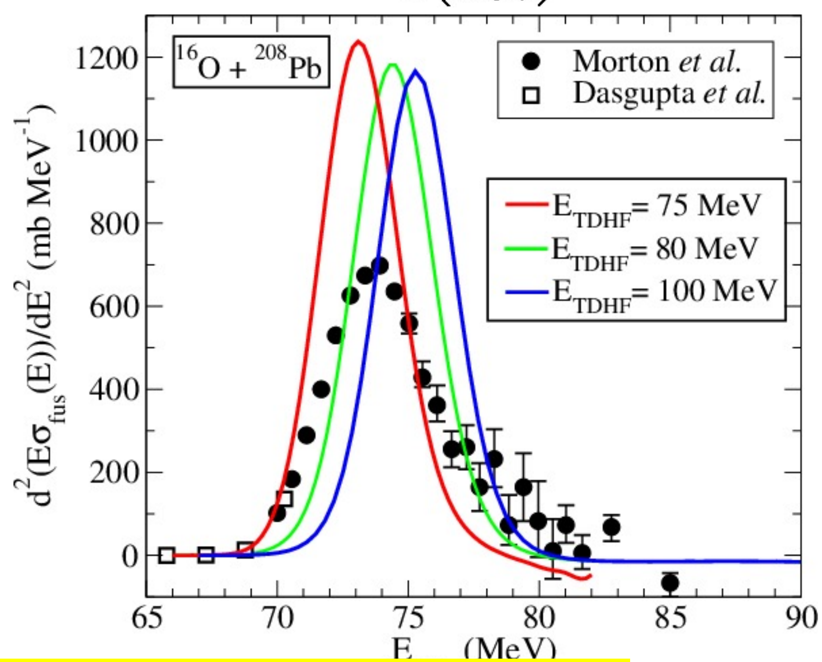






M(R)

K. Hagino and Y. Watanabe, PRC 76 (2007)



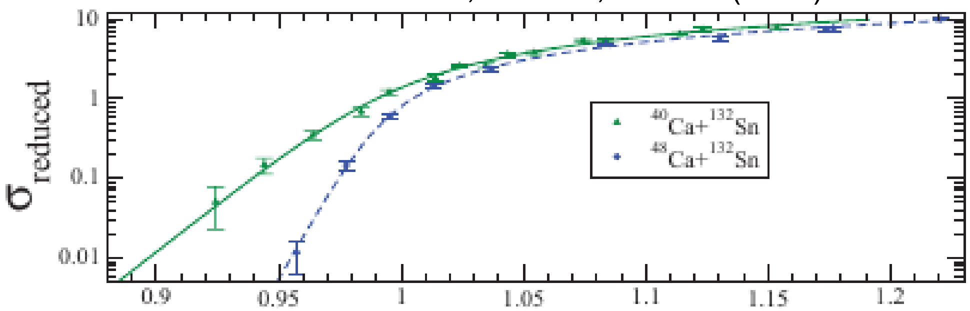
?

A. S. Umar, C. Simenel, and V. E. Oberacker, Phys. Rev. C **89**, 034611 (2014)

Neutron-Rich Systems ^{132,124}Sn+^{40,48}Ca

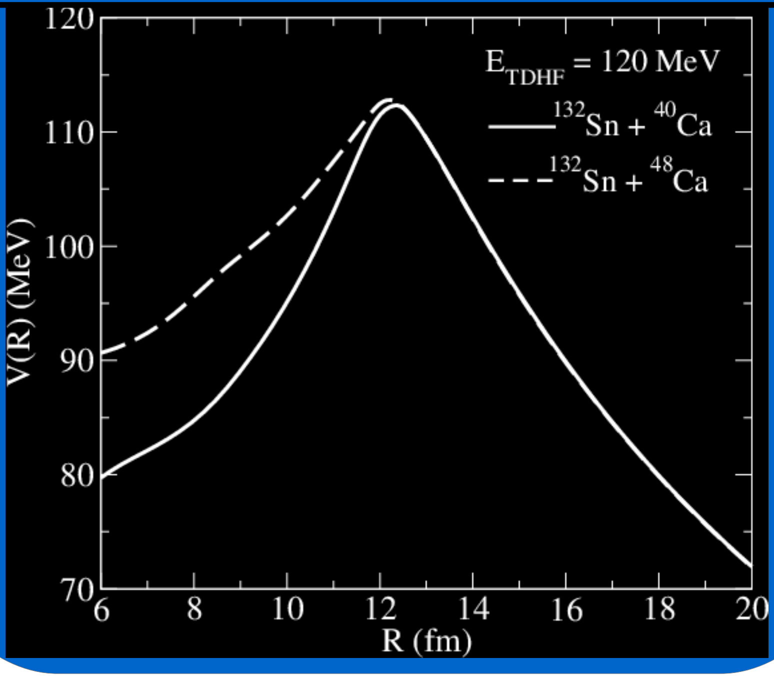
- Anomaly in sub-barrier fusion enhancement of ^{132}Sn+^{40}Ca versus ^{132}Sn+^{48}Ca
- Fusion enhancement not proportional to neutron pick-up Q-values

J.J. Kolata *et al.*, PRC 85, 054603 (2012)



- Barriers for both systems have similar heights
- ^{132}Sn+^{40}Ca barrier is narrower

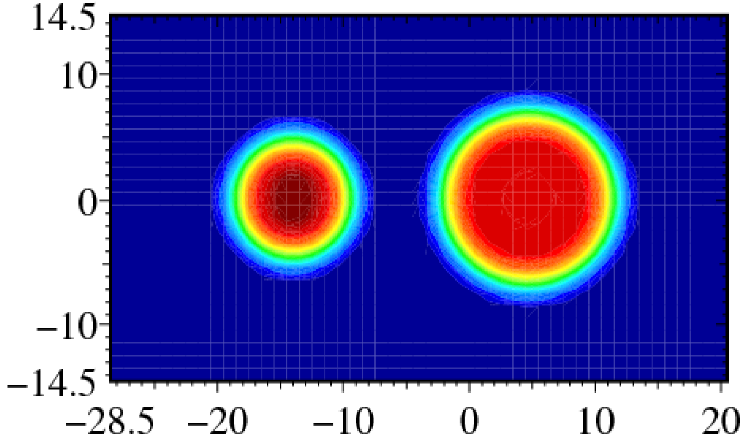
^{132}Sn+^{40}Ca versus ^{132}Sn+^{48}Ca Potentials



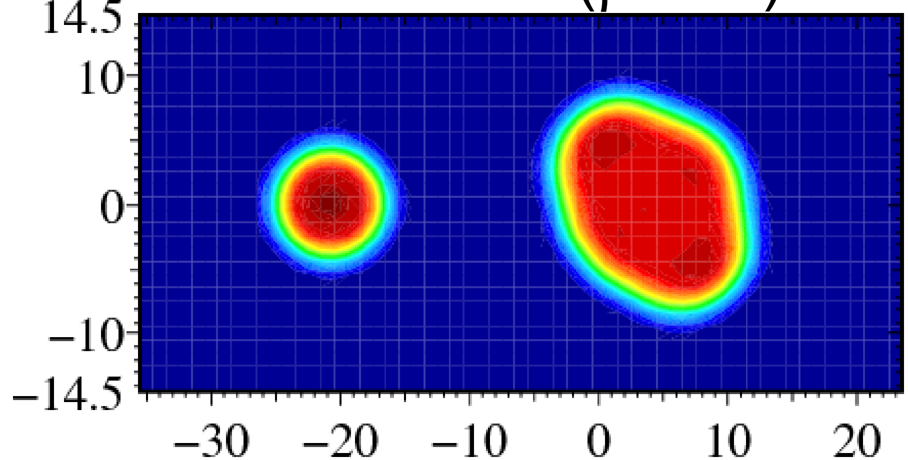
V.E. Oberacker, A.S. Umar, J.A. Maruhn, and P.-G. Reinhard, PRC **85**, 034609 (2012)
V.E. Oberacker and A.S. Umar, PRC **87**, 034611 (2013)

Cold and Hot Fusion of Heavy Systems

$^{70}Zn+^{208}Pb$



$^{48}Ca+^{238}U$ (β=45°)



Heavy nuclei exhibit a very different behavior in forming a composite system

Light-Medium Mass Systems

$$\sigma_{capture} \approx \sigma_{ER} \approx \sigma_{fusion}$$

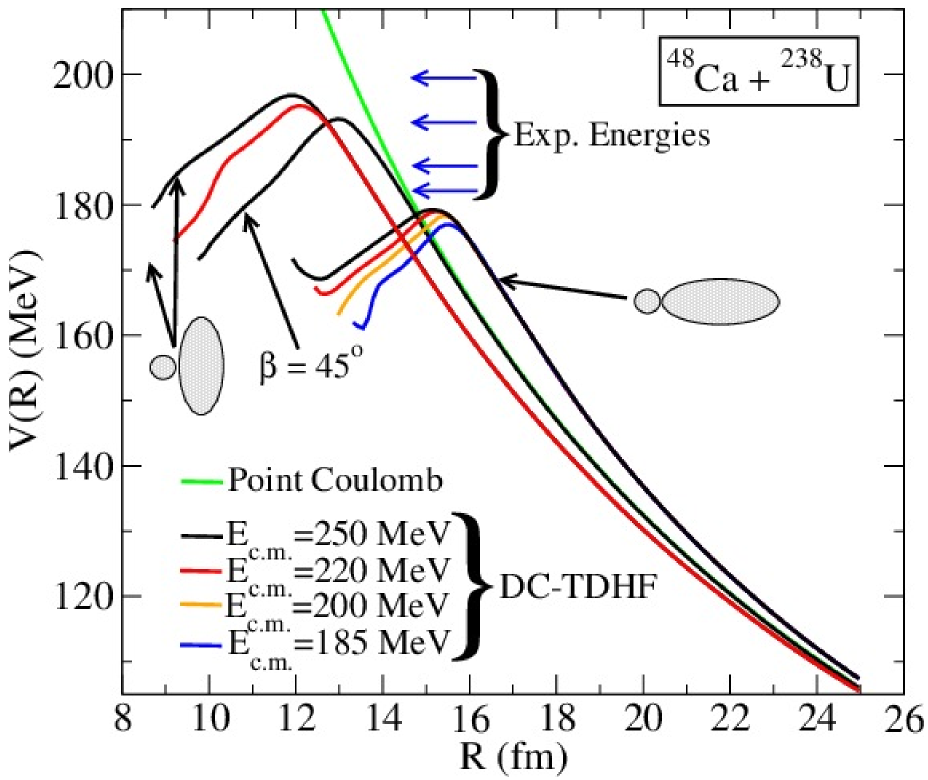
- Fission and quasi-fission negligible
- Simple V(R) for composite system
- Small energy dependence

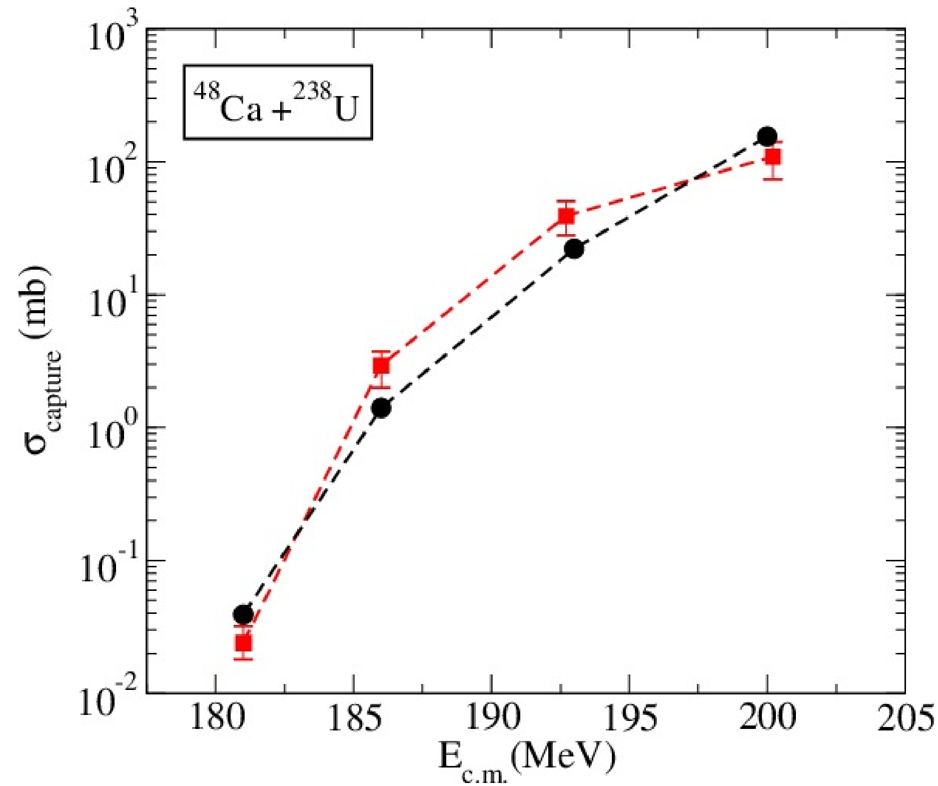
Heavy Systems

$$\sigma_{capture} = \sigma_{QF} + \sigma_{FF} + \sigma_{ER}$$

- Quasi-fission dominant
- Di-nuclear composites common
- A multi-stage V(R)

Capture for ^{48}Ca+^{238}U





Experimental data:

1. M. G. Itkis et al., J. Nucl. Radiochem. Sci. 3, **57** (2002)
2. M. G. Itkis et al., Nucl. Phys. A **734** , 136 (2004)

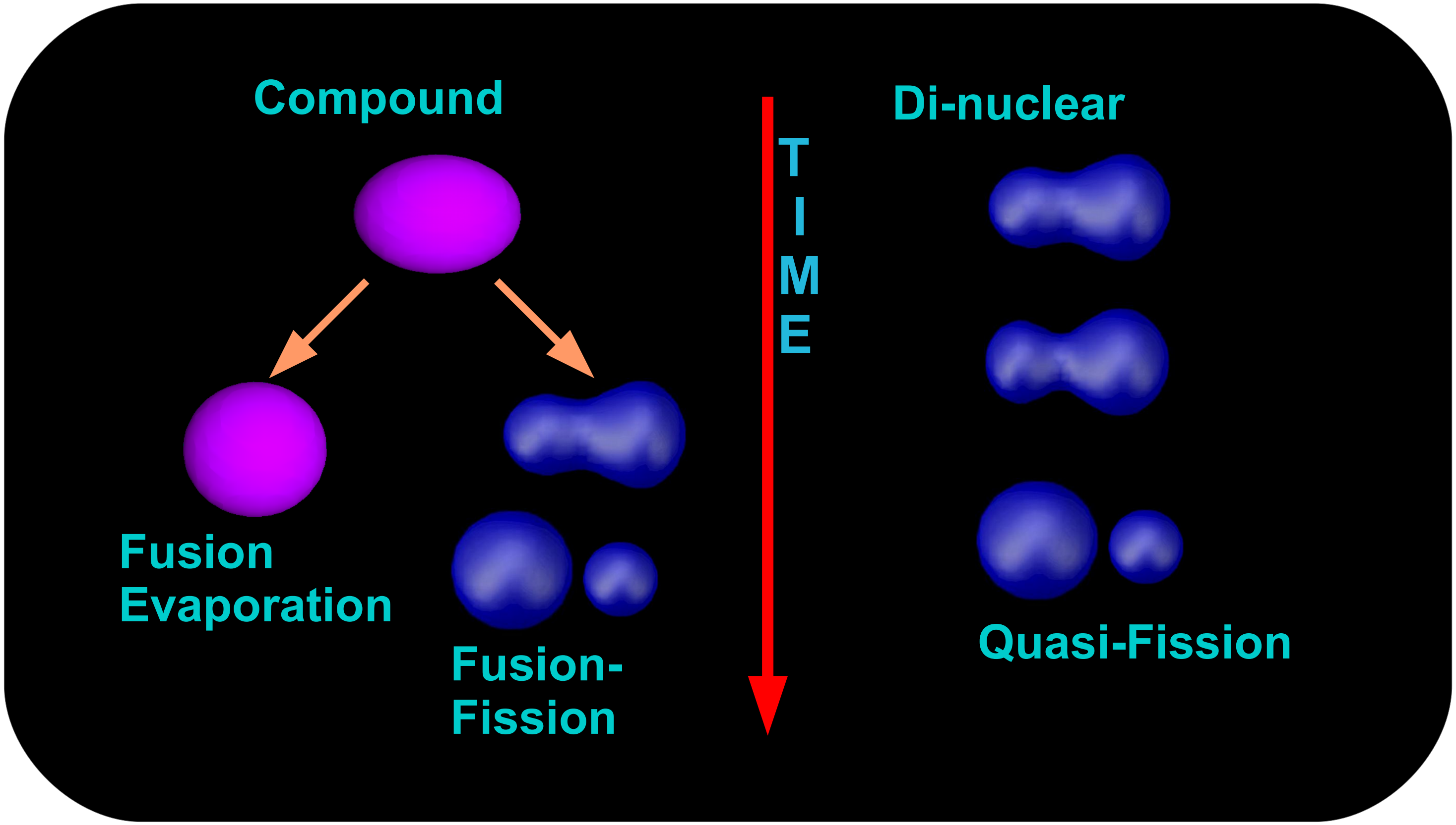
Angle average ^{238}U alignment

- x-section falls rapidly for β>10°
- sin(β) multiply small angles
- P(β) is in the range 0.4-0.6

$$\sigma_f(E_{c.m.}) = \int_0^1 d\beta \sin(\beta) P(\beta) \sigma(E_{c.m.}, \beta)$$

A.S. Umar, V.E. Oberacker, J.A. Maruhn, and P.-G. Reinhard, PRC **81**, 064607 (2010)

Study of Quasifission with TDHF

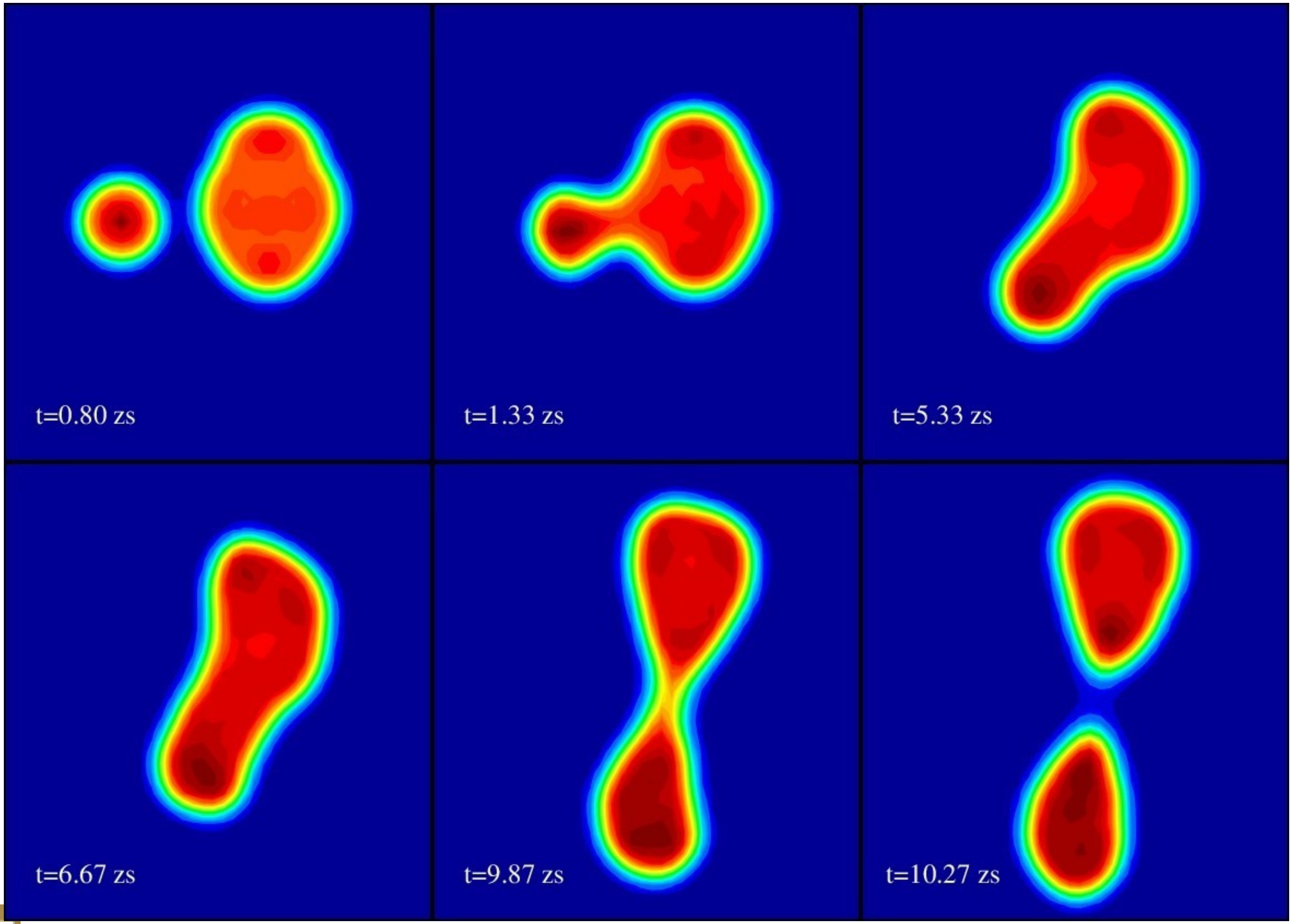


Quasifission in – $^{40,48}Ca + ^{238}U$

Heavy Systems

$$\sigma_{capture} = \sigma_{QF} + \sigma_{fusion-fission} + \sigma_{ER}$$

- QF dominant part
- Important for studying SHE dynamics



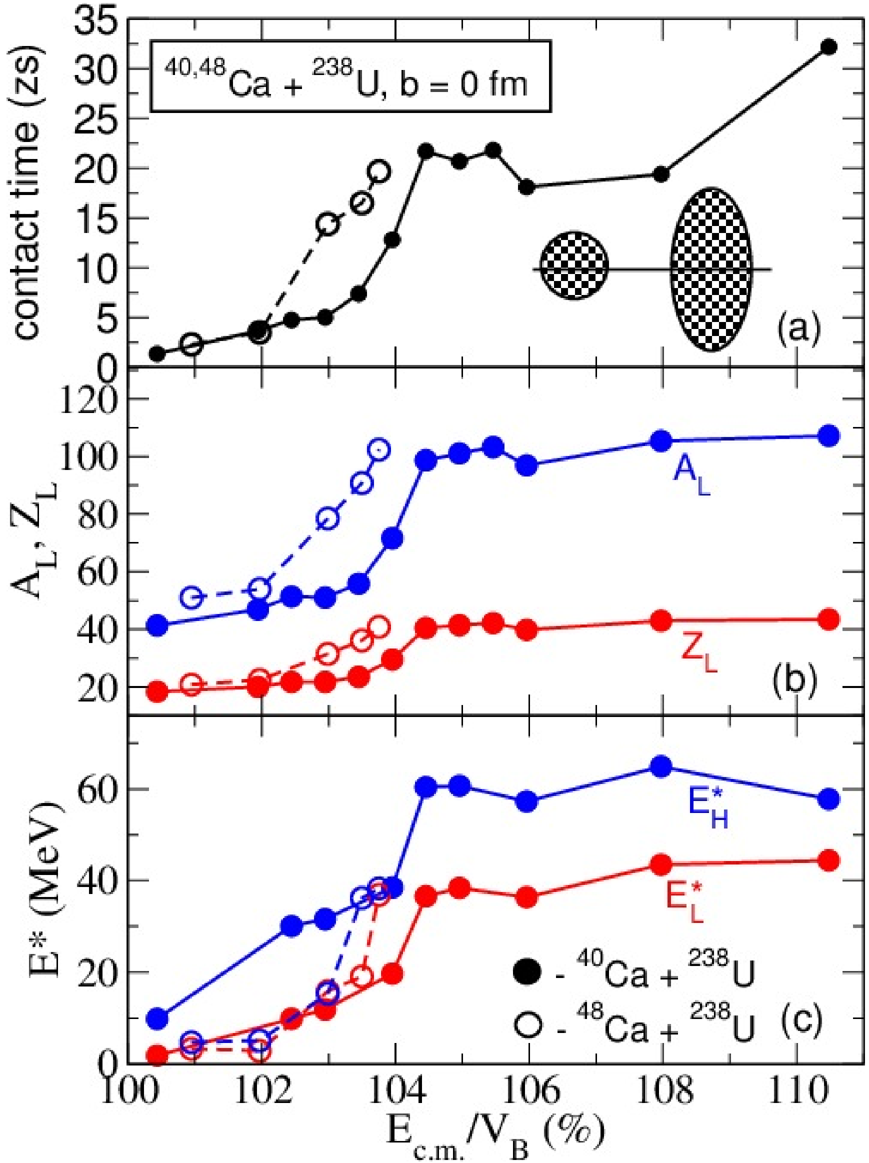
Final masses:
$A_L = 101$, $A_R = 177$
$Z_L = 41$, $Z_R = 71$

$E_{cm} = 209$ MeV
b=1.103fm (L=20)

$^{40}Ca + ^{238}U$

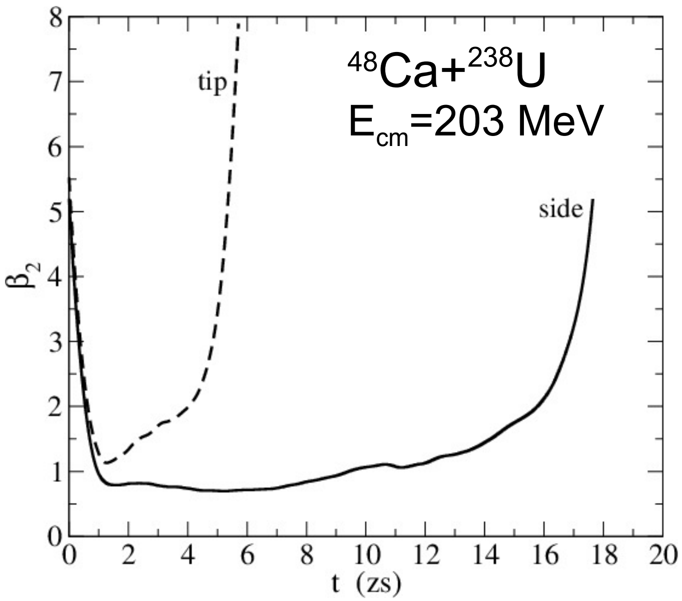
V.E. Oberacker, A.S. Umar, C. Simenel, PRC **90**, 054605 (2014)

Quasifission – $^{40,48}Ca+^{238}U$



- Compare $^{40,48}Ca+^{238}U$ (b=0)
- **fusion** implies contact-time > 35 zs (plus density shows no indication of QF)
- $^{40}Ca+^{238}U$ wider energy range for QF
- E* sharing seems different (calculated dynamically using DC-TDHF)

Each point takes about a week on a 16 processor workstation

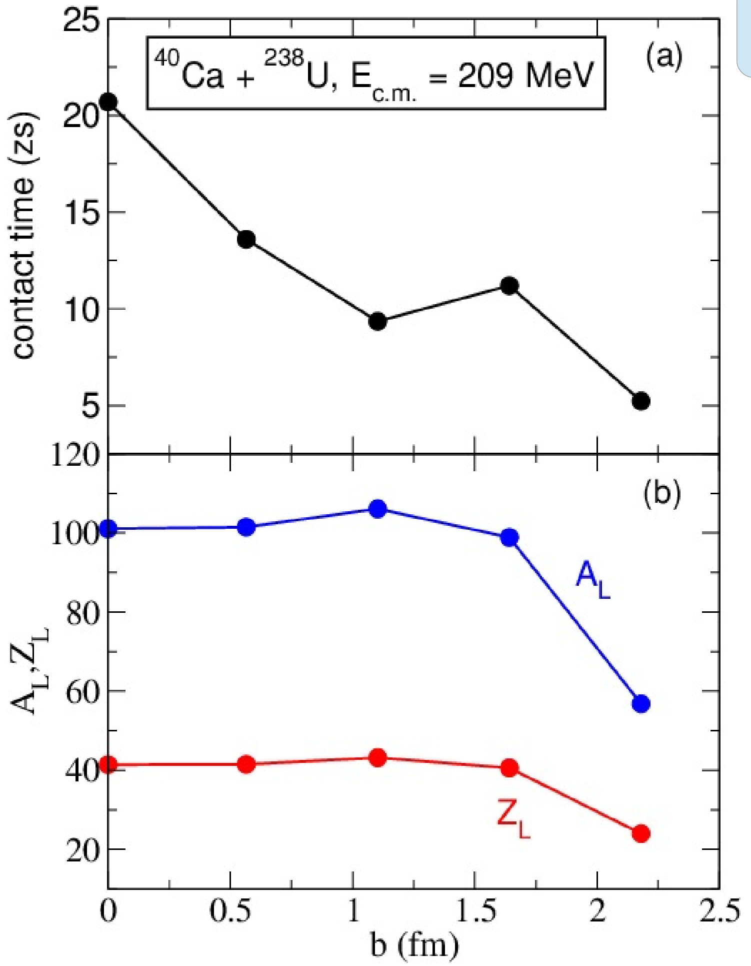


$$\beta_2 = \frac{4\pi}{3}\frac{Q_{20}}{AR_0^2}$$

The β=0° orientation of ^{238}U results in much smaller contact-times and mass transfer

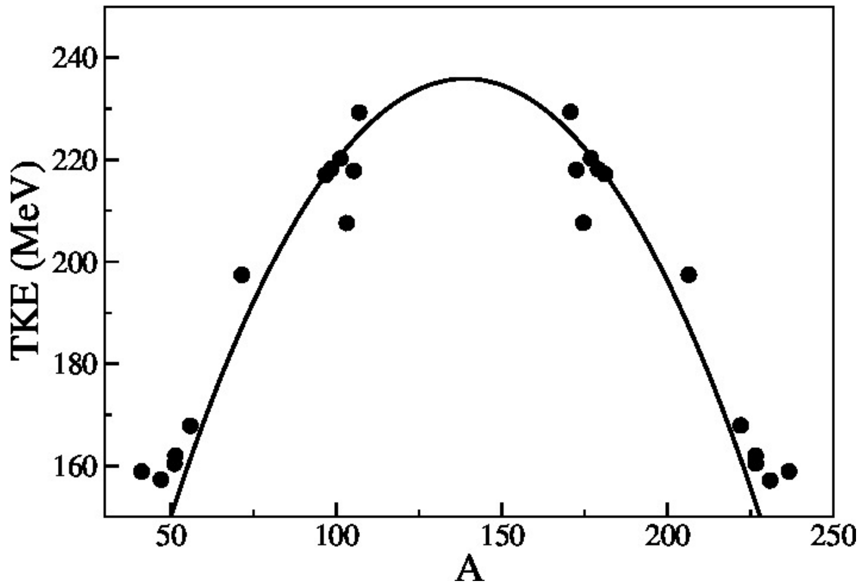
V.E. Oberacker, A.S. Umar, C. Simenel, PRC **90**, 054605 (2014)

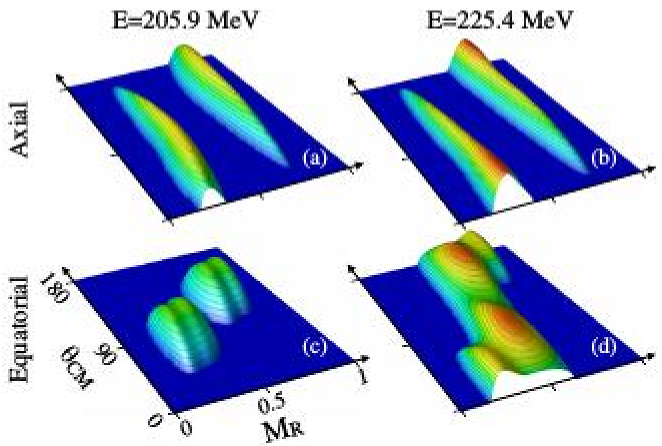
Impact Parameter Dependence – Viola Systematics



Narrow range of impact parameters at low energies

Final fragment TKE's well described by Viola systematics



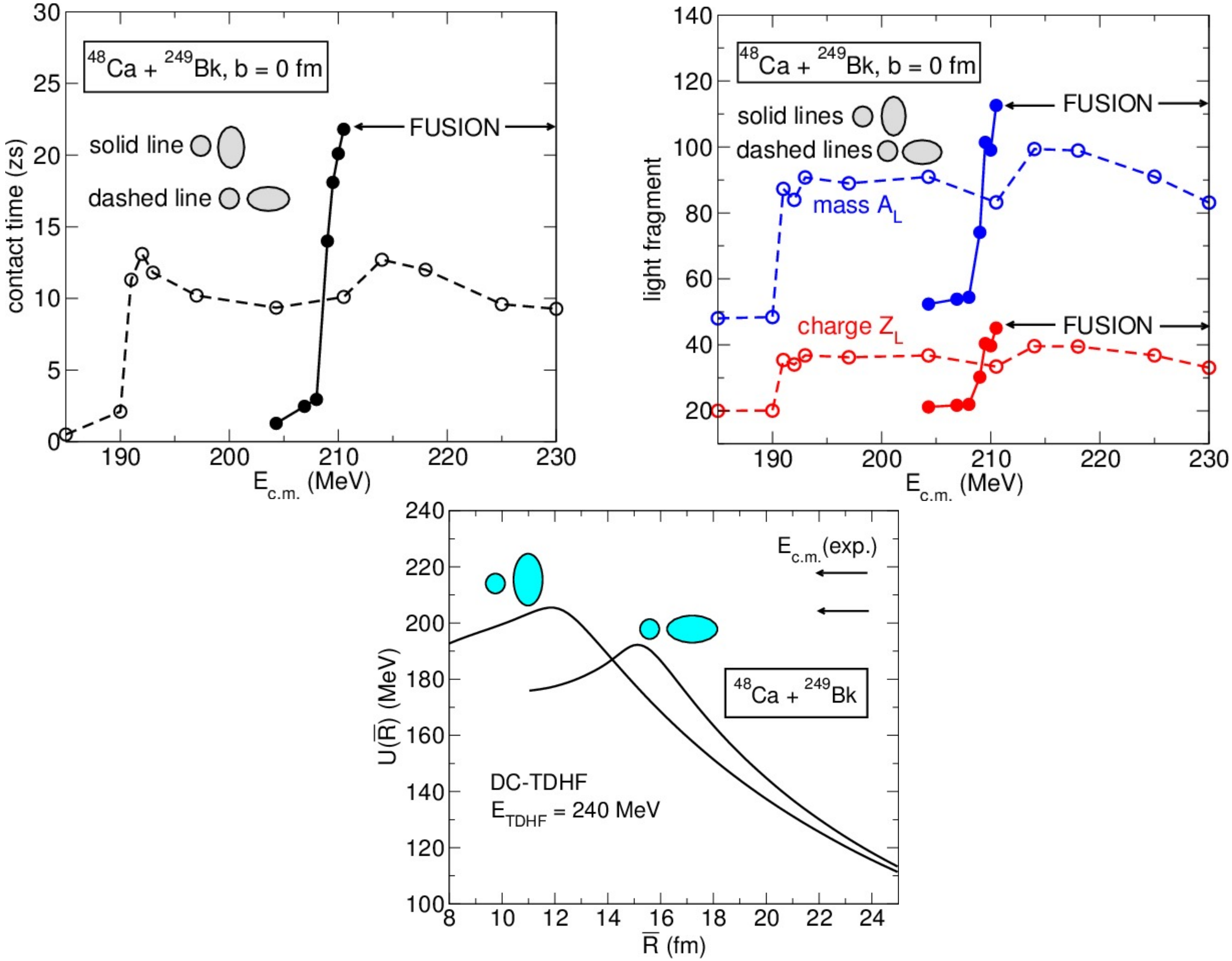


^{40}Ca + ^{238}U

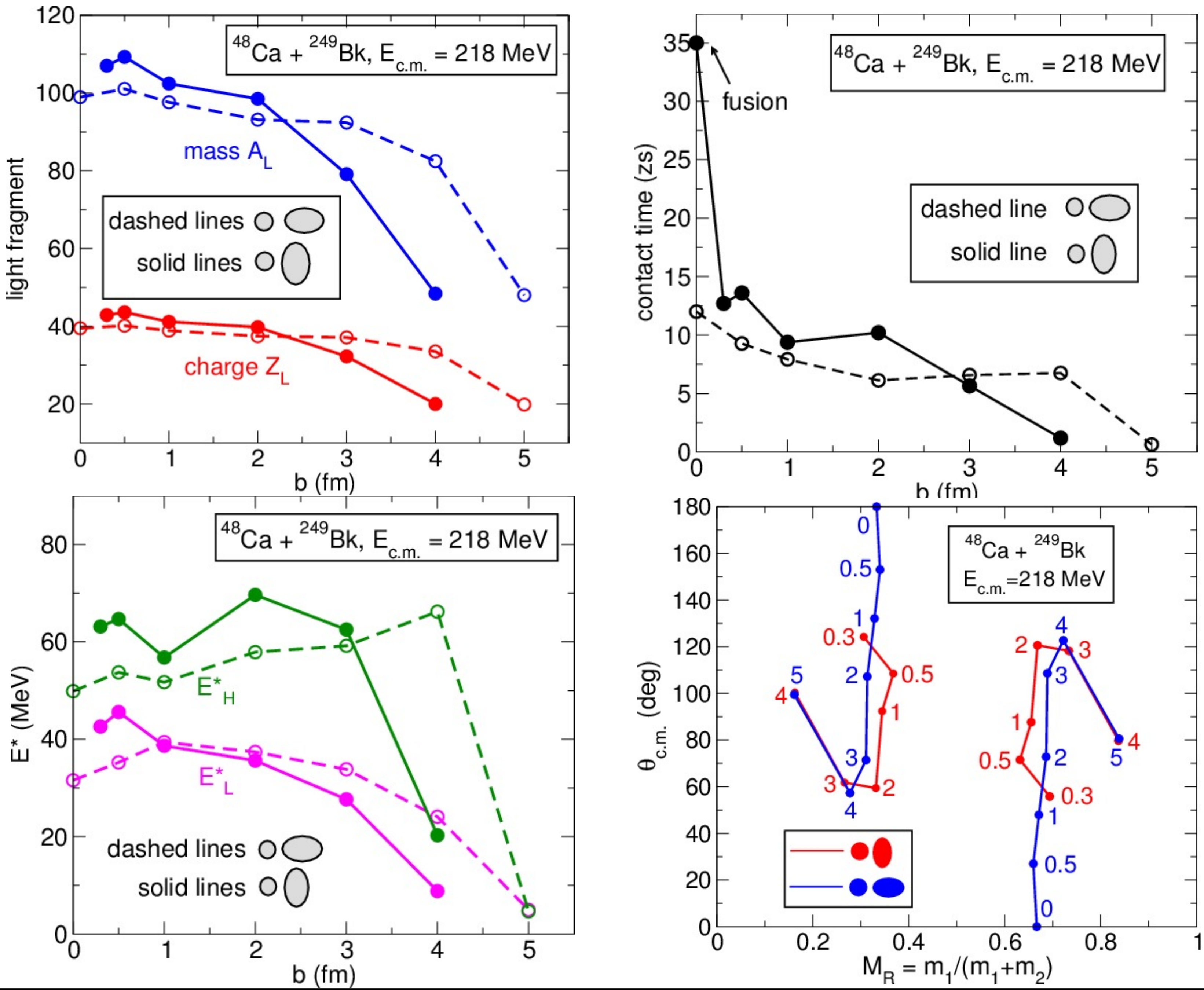
Wakhle et al., **PRL** 113, 182502 (2014)

V.E. Oberacker, A.S. Umar, C. Simenel, PRC **90**, 054605 (2014)

Quasifission in $^{48}Ca+^{249}Bk$ (to be published)

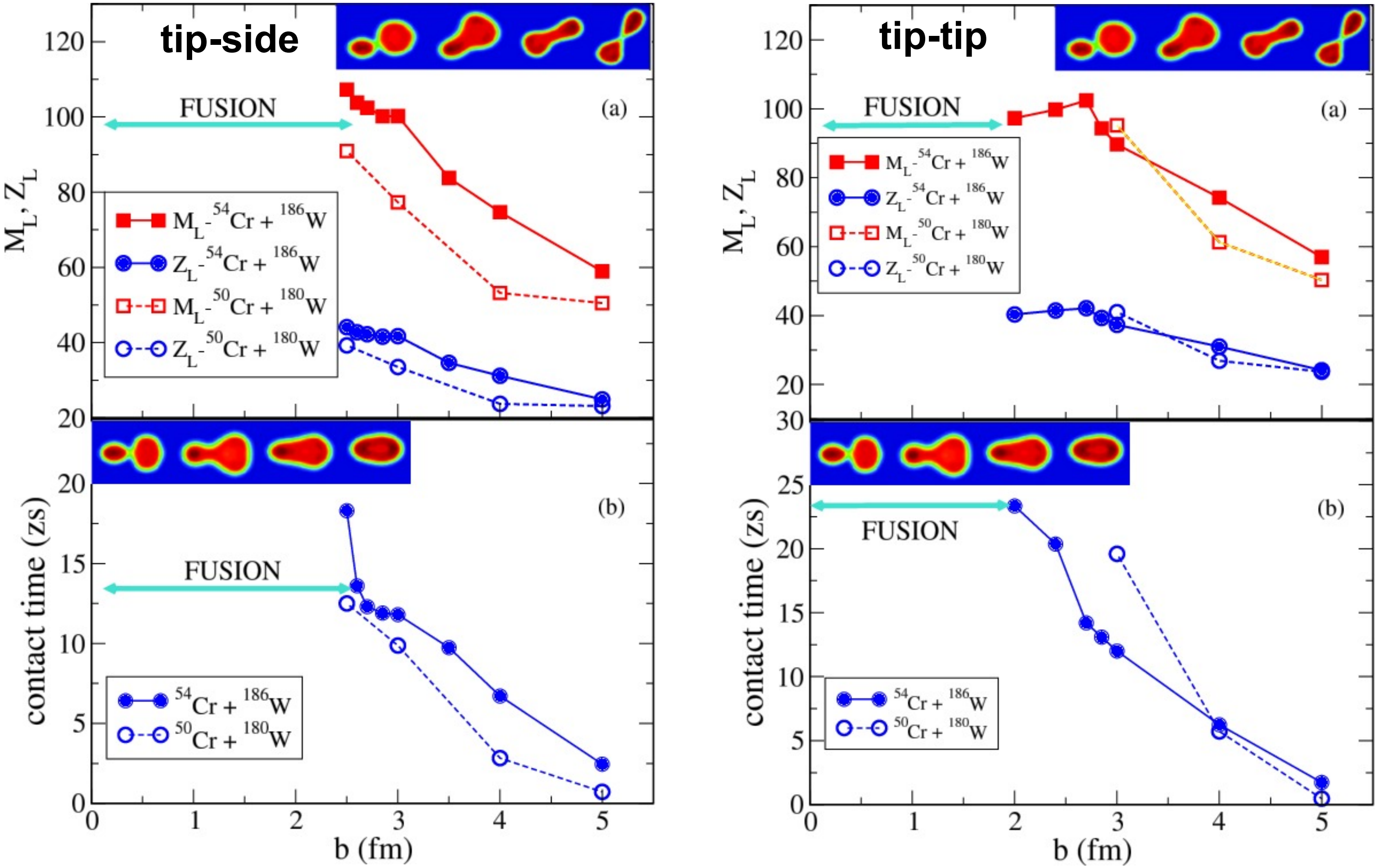


Quasifission in $^{48}Ca+^{249}Bk$ ($E_{c.m.}$ = 218 MeV)



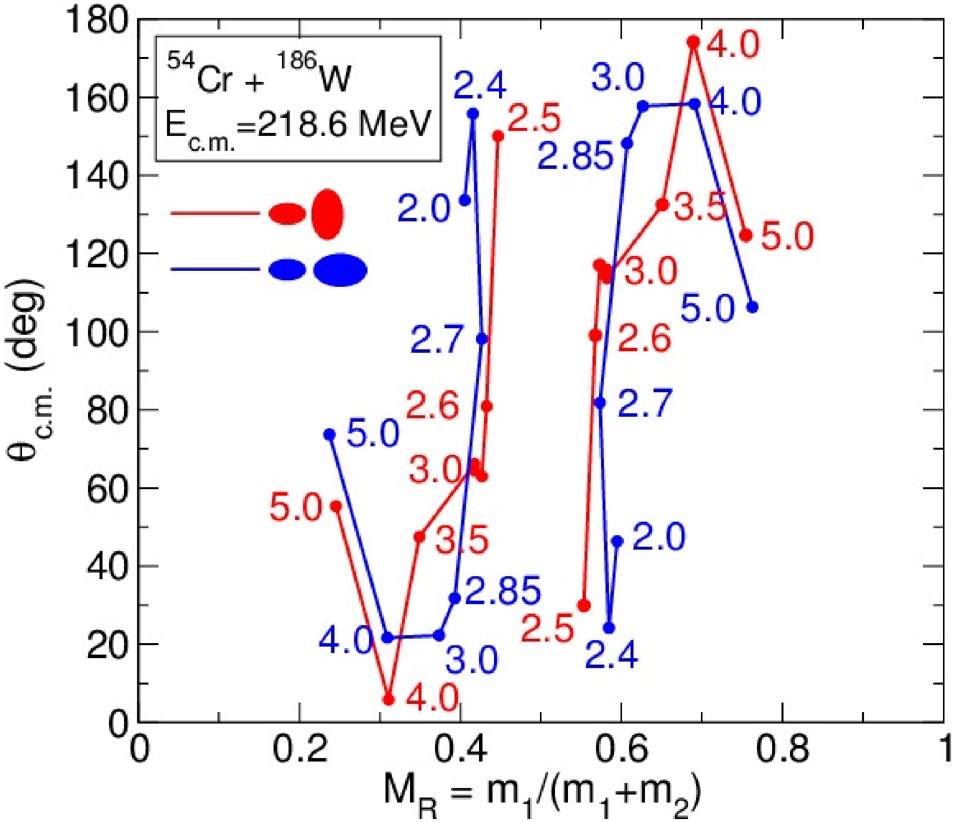
Quasifission in $^{50,54}Cr+^{180,186}W$ ($E_{c.m.}/V_B$=1.13)

Two deformed nuclei with smaller mass/charge asymmetry than Ca+U

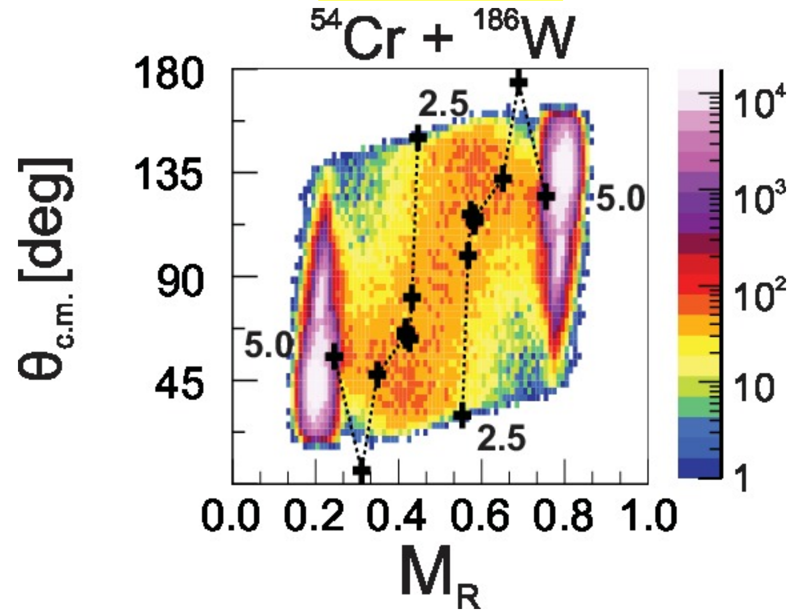


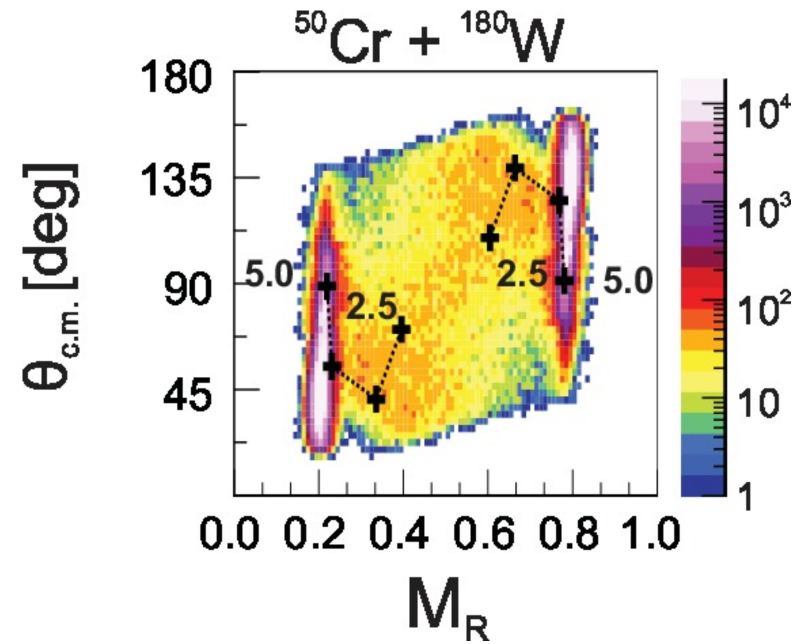
K. Hammerton, Z. Kohley, D. J. Hinde, M. Dasgupta, A. Wakhle, E. Williams,V. E. Oberacker, A. S. Umar, I. P. Carter, K. J. Cook, J. Greene, D. Y. Jeung, D. H. Luong, S. D. McNeil, C. S. Palshetkar, D. C. Rafferty, C. Simenel, and K. Stiefel, PRC **91**, 041601(R) (2015)

Mass Angle Distributions (MAD's)

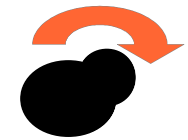


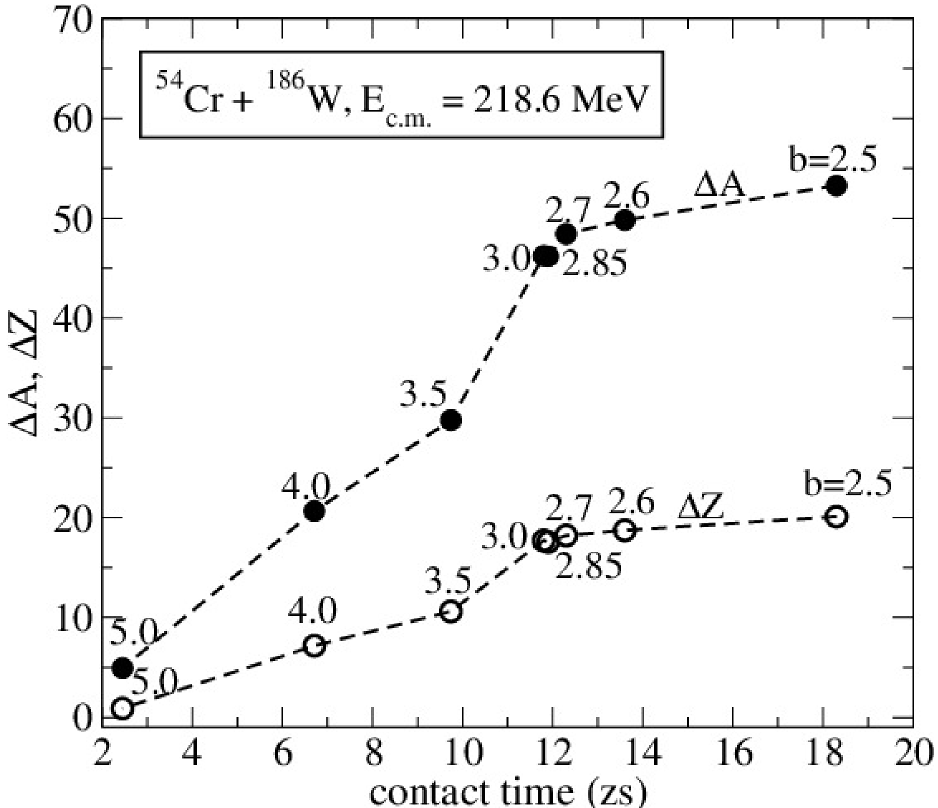
TIP-SIDE

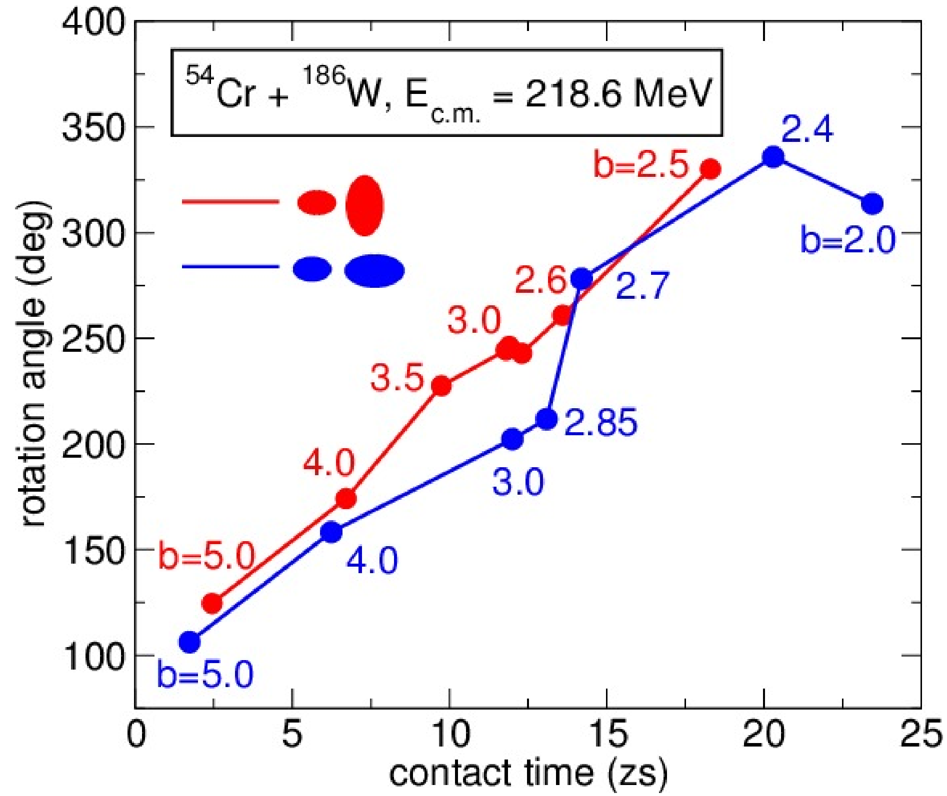




Contact Time versus Mass/Charge Transfer and Rotation Angle







Larger contact time → larger mass transfer

Larger contact time → larger rotation angle

Fission Fragment Angular Distributions - P_{CN}

- Angular distribution based on TSM (see Yanez *et al.* PRC 88, 014606 (2013))

$$W(\theta) = \sum_{J=0}^{J_{CN}} \frac{(2J+1)^2 exp[-(J+1/2)^2 sin^2\theta/4K_0^2(FF)] J_0[i(J+1/2)^2 sin^2\theta/4K_0^2(FF)]}{erf[(J+1/2)/(2K_0^2(FF))^{1/2}]}$$
$$+ \sum_{J=J_{CN}}^{J_{\max}} \frac{(2J+1)^2 exp[-(J+1/2)^2 sin^2\theta/4K_0^2(QF)] J_0[i(J+1/2)^2 sin^2\theta/4K_0^2(QF)]}{erf[(J+1/2)/(2K_0^2(QF))^{1/2}]}$$

QF angular distribution

- Parameter K_0 involves shape and temperature

$$K_0^2 = T\Im_{eff}/\hbar^2$$

$$P_{CN} \approx \frac{\sigma_{FF}}{\sigma_{QF} + \sigma_{FF}}$$

- Need parallel/perpendicular moment of inertia

$$\frac{1}{\Im_{eff}} = \frac{1}{\Im_{\parallel}} - \frac{1}{\Im_{\perp}}$$

- Assumption!

$$\Im_0/\Im_{eff} = 1.5$$

?

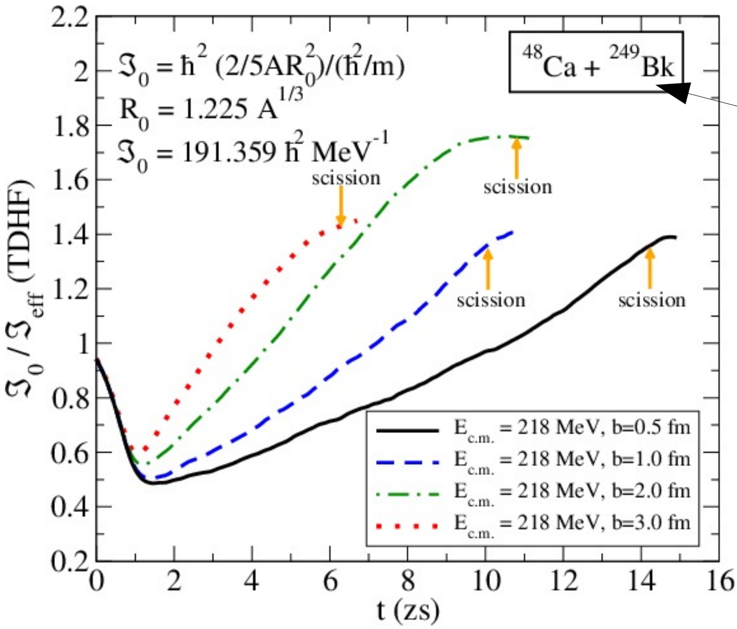
- Temperature at the <u>saddle</u> point

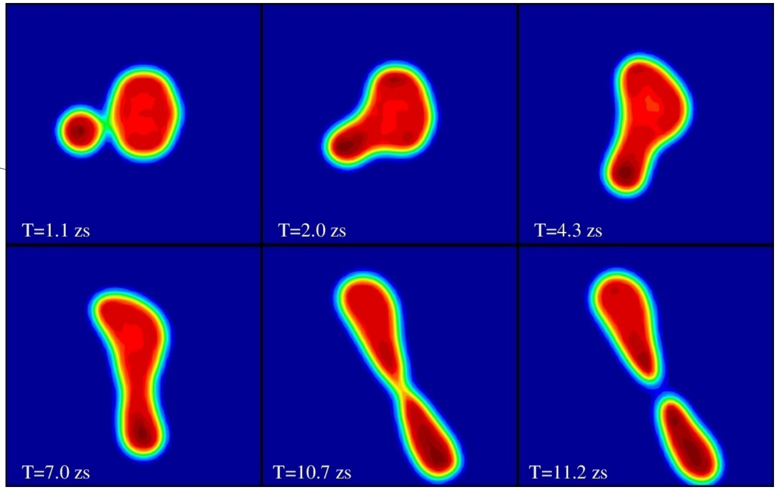
$$\mathcal{T} = \left[\frac{E^* - B_f - E_{rot} - E_\nu}{A/8.5}\right]^{1/2}$$

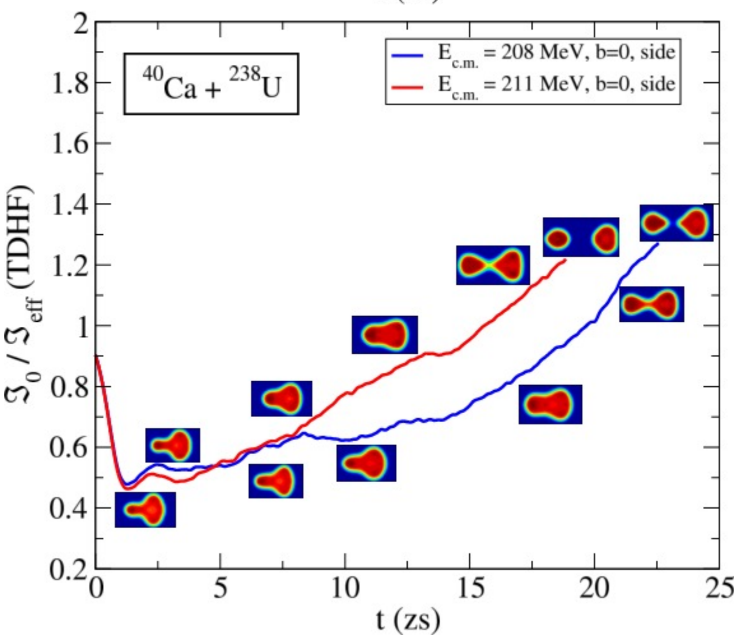
- Can obtain from <u>dynamical</u> E* using DC-TDHF

$$\mathcal{T} = \left[\frac{E^*_{TDHF}}{A/8.5}\right]^{1/2}$$

Moment of Inertia from TDHF







- Diagonalize the moment of inertia tensor

$$\Im_{ij}/m = \int d^3r\ \rho_{TDHF}(\mathbf{r},t)(r^2\delta_{ij} - x_i x_j)$$

- Eigenvalues give the parallel/perpendicular moment of inertia

$$\frac{1}{\Im_{eff}} = \frac{1}{\Im_{\|}} - \frac{1}{\Im_{\perp}}$$

- Ratio $\Im_0/\Im_{eff}$

$$\Im_0 = \hbar^2(2/5AR_0^2)/(\hbar^2/m)$$

Equivalent sphere

A.S. Umar, V.E. Oberacker, and C. Simenel, Phys. Rev. C 92, 024601 (2015)

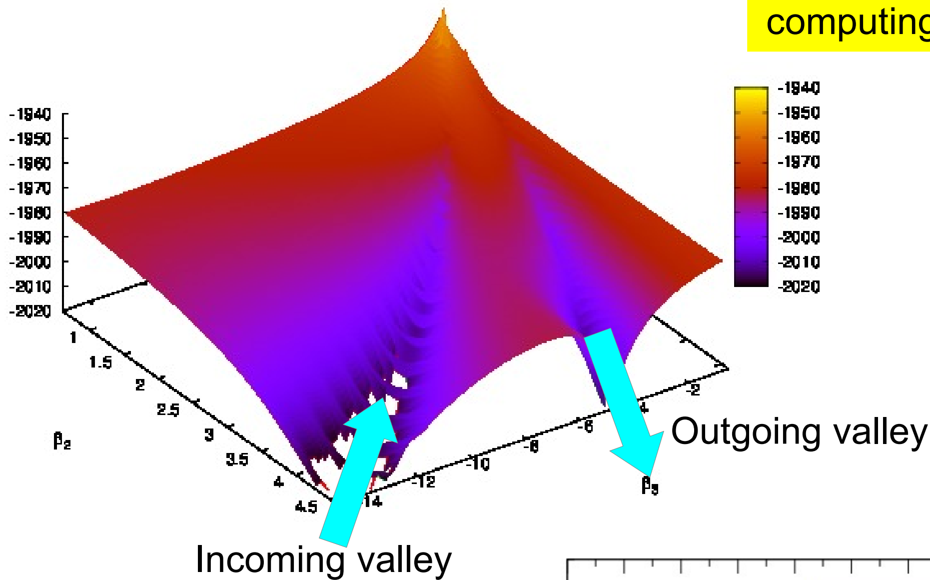
Collective Dynamics with DC-TDHF

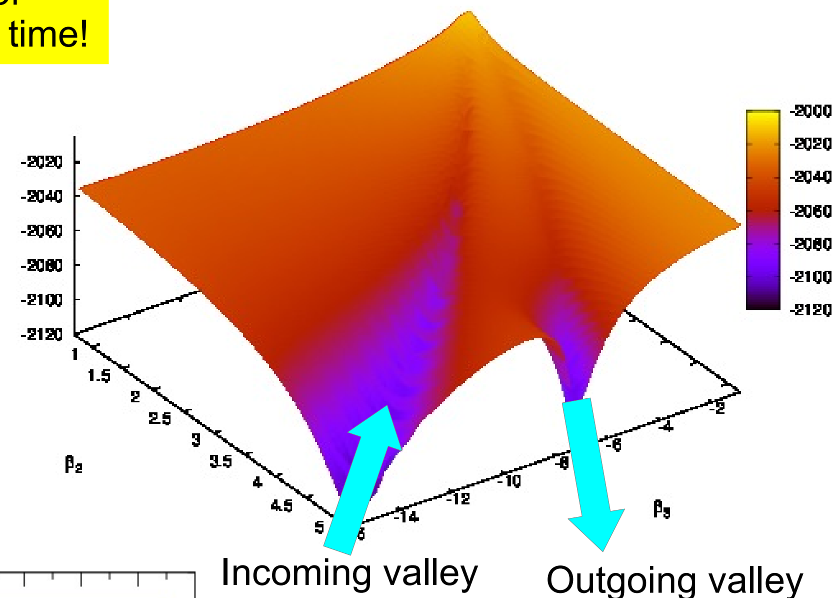
- Obtain collective surface seen by TDHF using dynamical density as a constraint

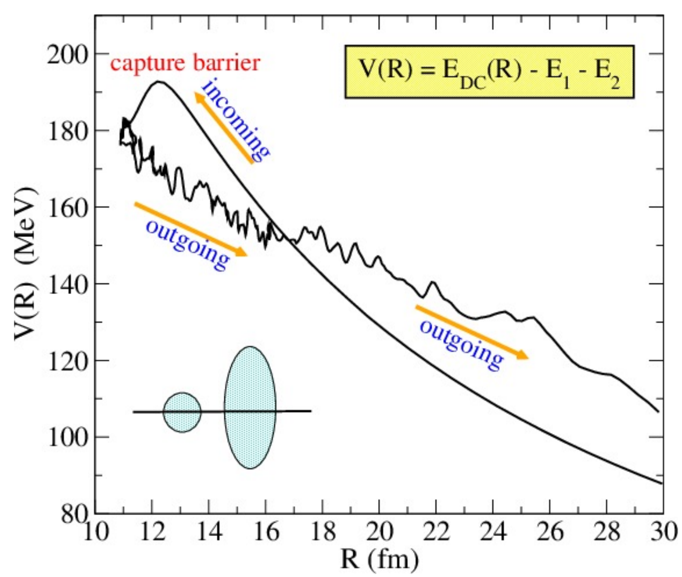
$^{40}Ca + ^{238}U$

2 months of computing time!

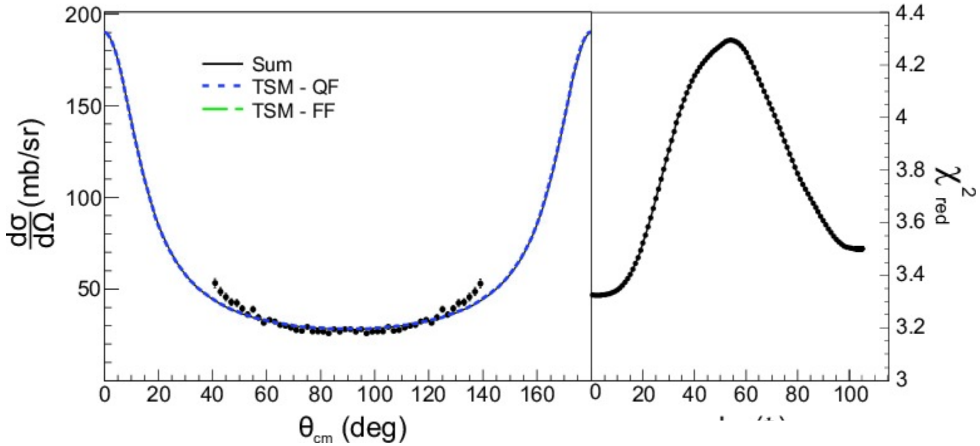
$^{48}Ca + ^{238}U$

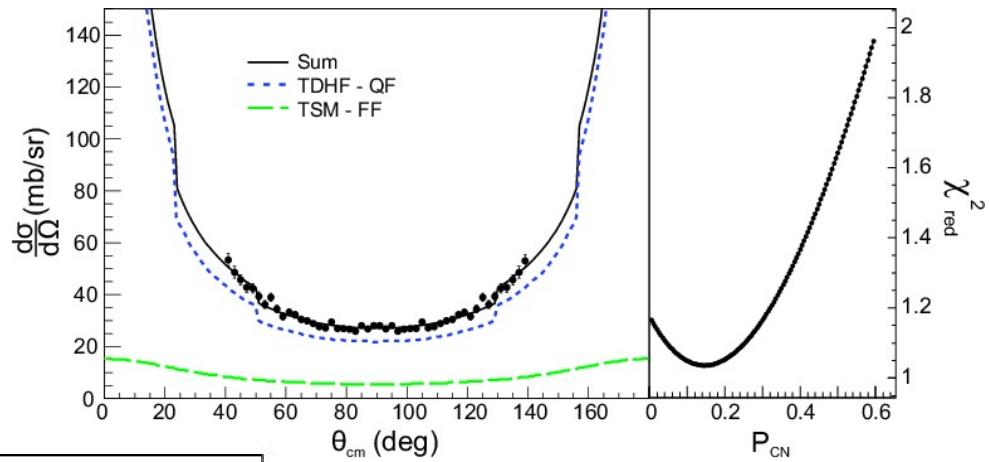


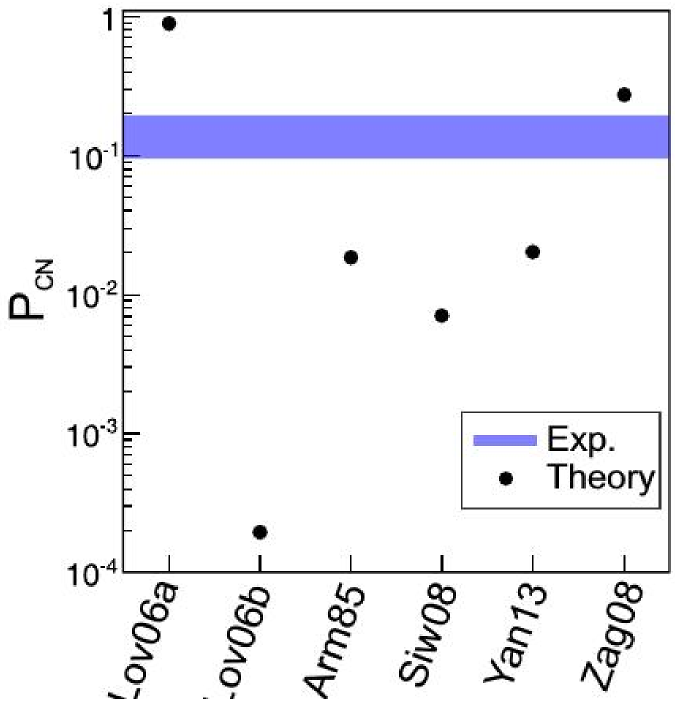




PCN from TDHF Angular Distributions



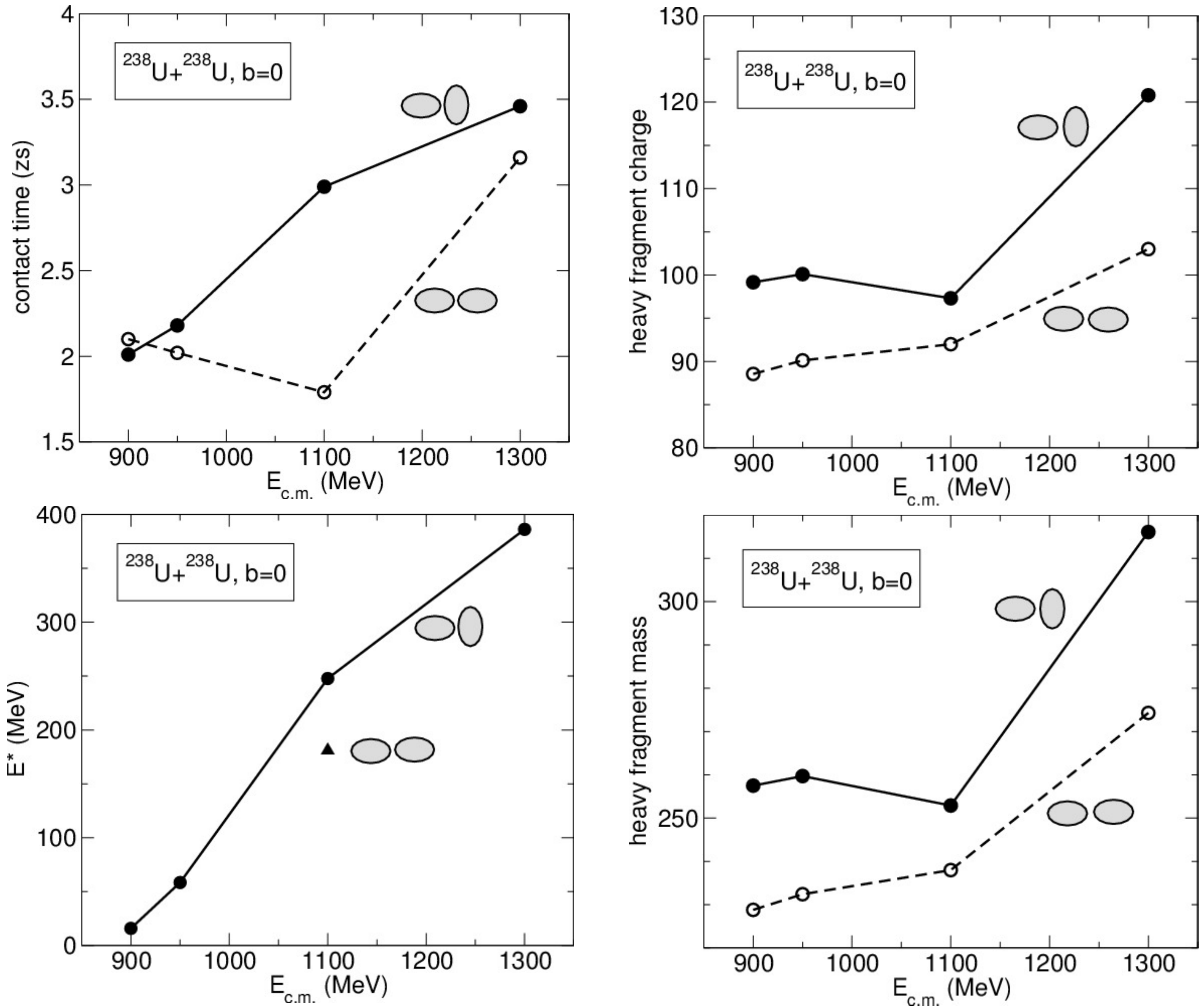




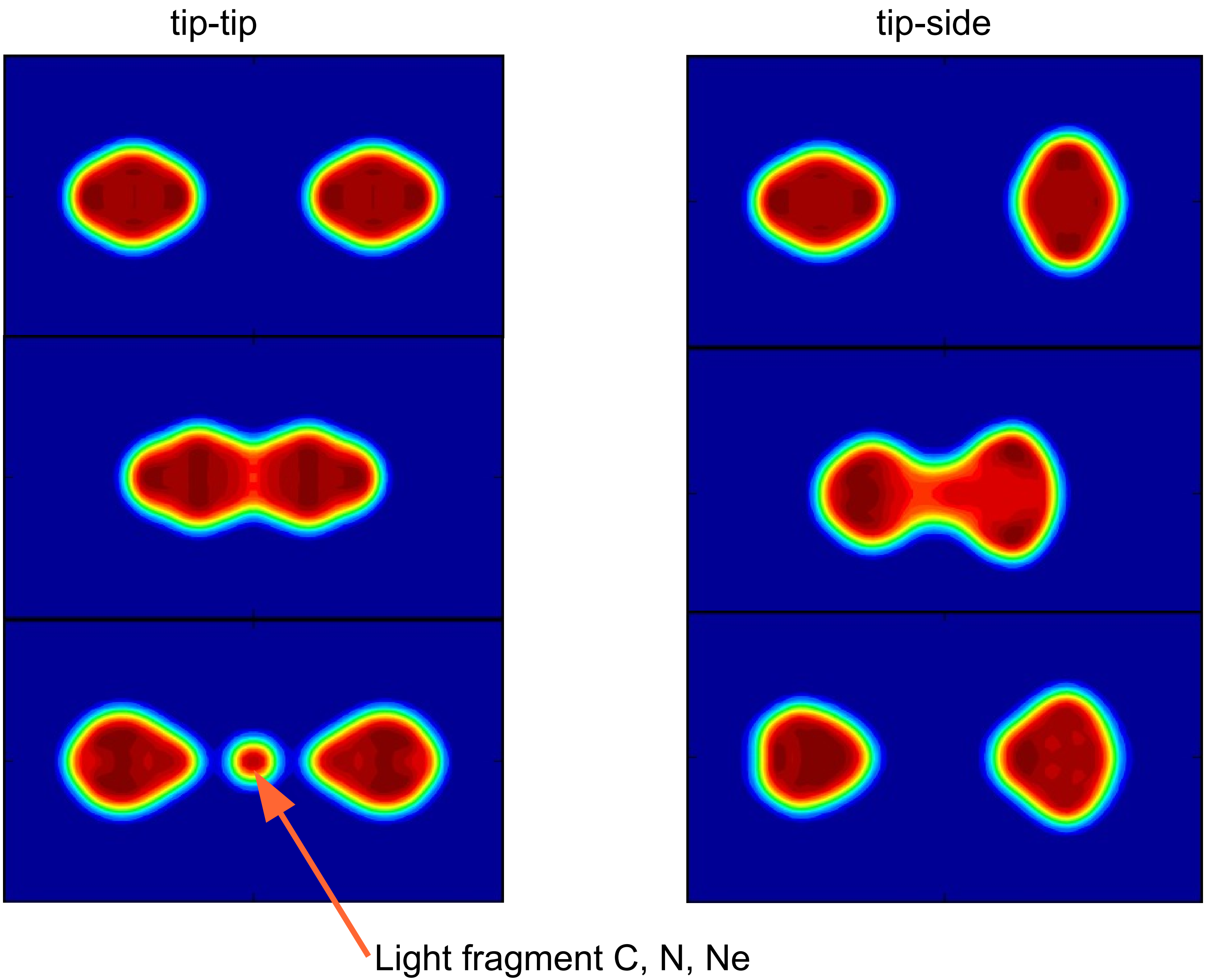
Comparison with different models

Z. Kohley, private communication

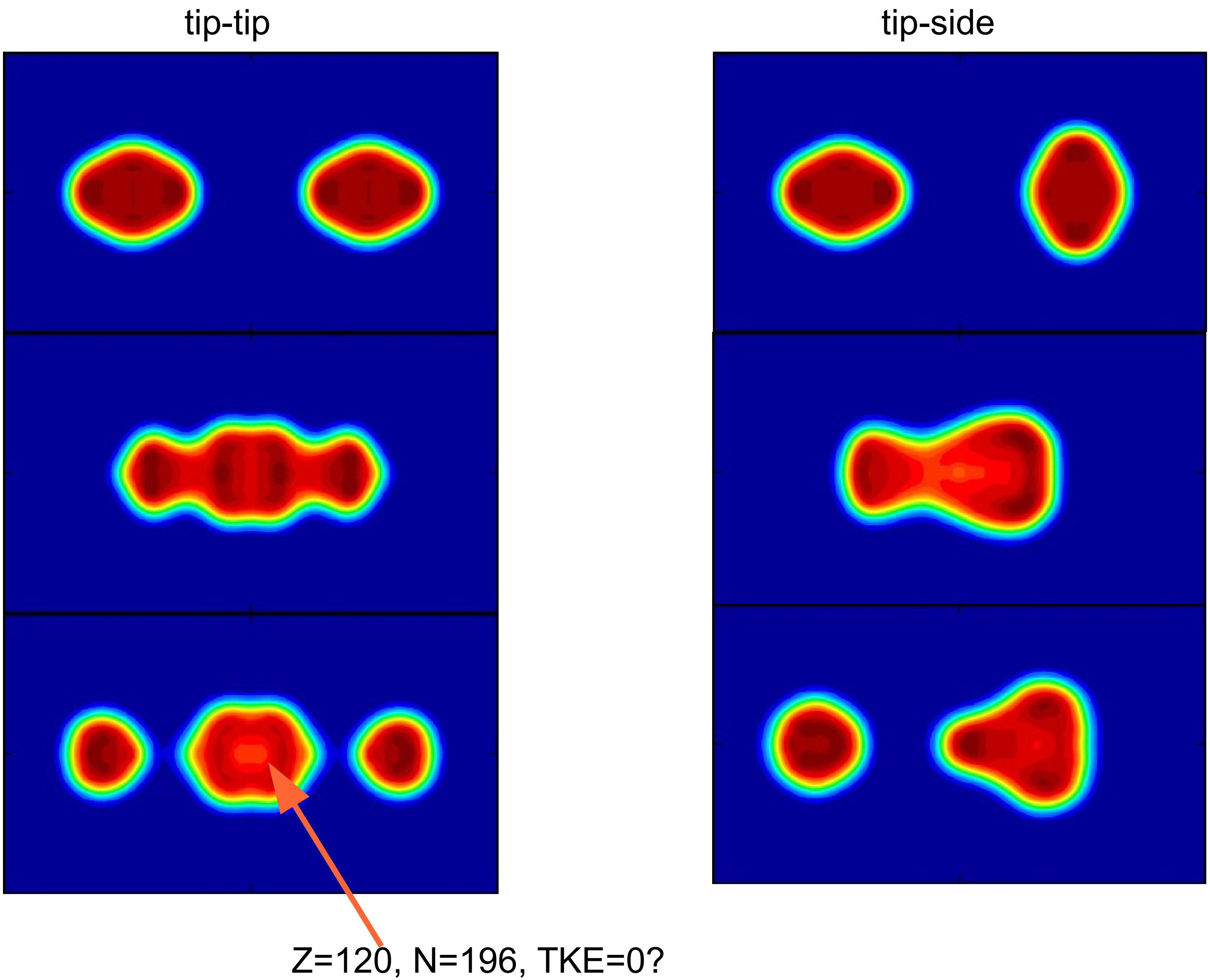
$^{238}U+^{238}U$ (b=0, preliminary results)



$^{238}U + ^{238}U$ at Ecm = 900 MeV



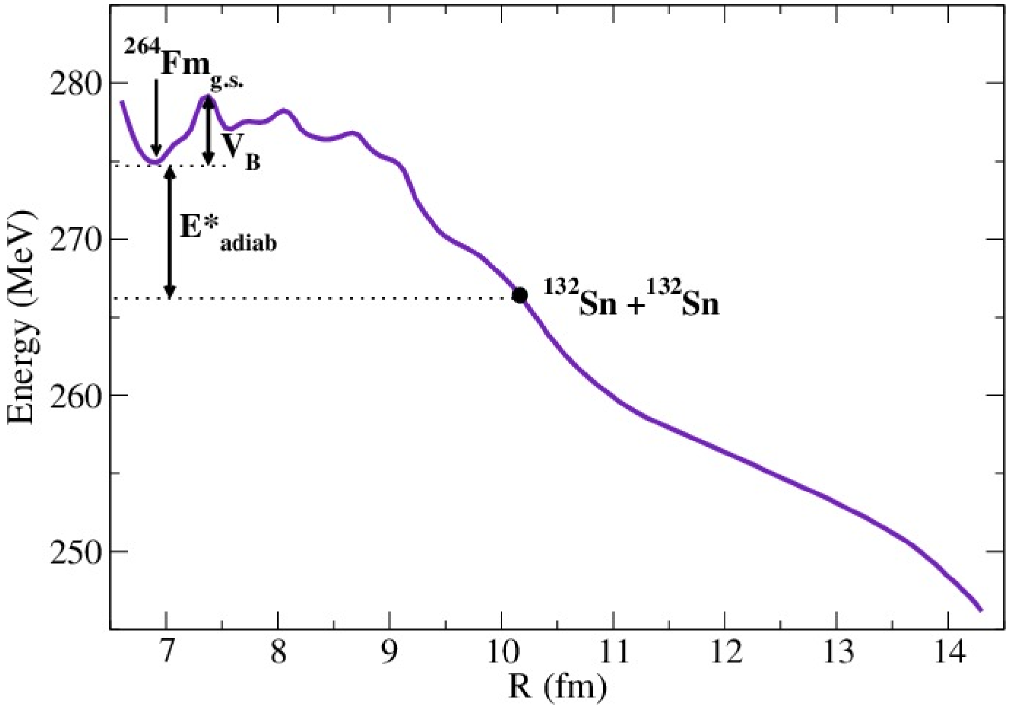
$^{238}U+^{238}U$ Ecm = 1300 MeV

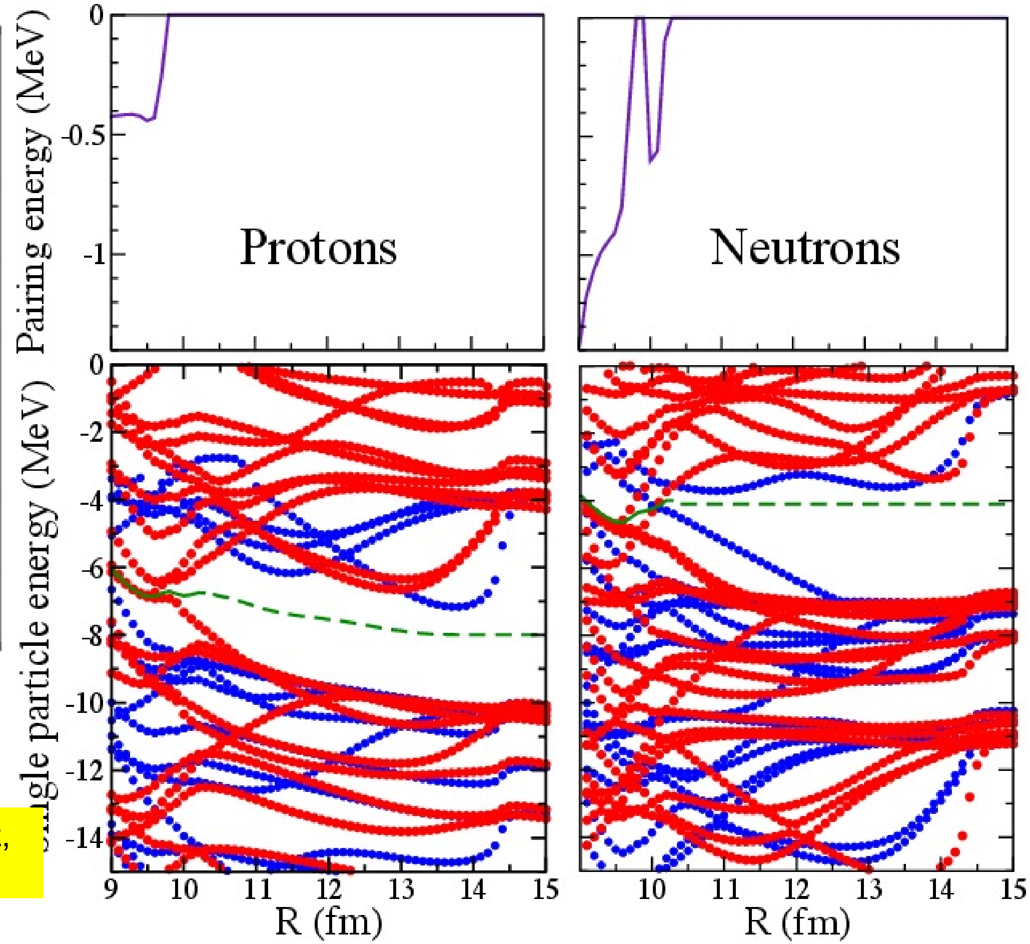


Scission Dynamics

Scission Dynamics Using TDHF – Fragment Pre-Formation

- Transition from adiabatic motion to non-adiabatic motion of scission
- Follow the single-particle states as a function of deformation, look for the last level crossing.



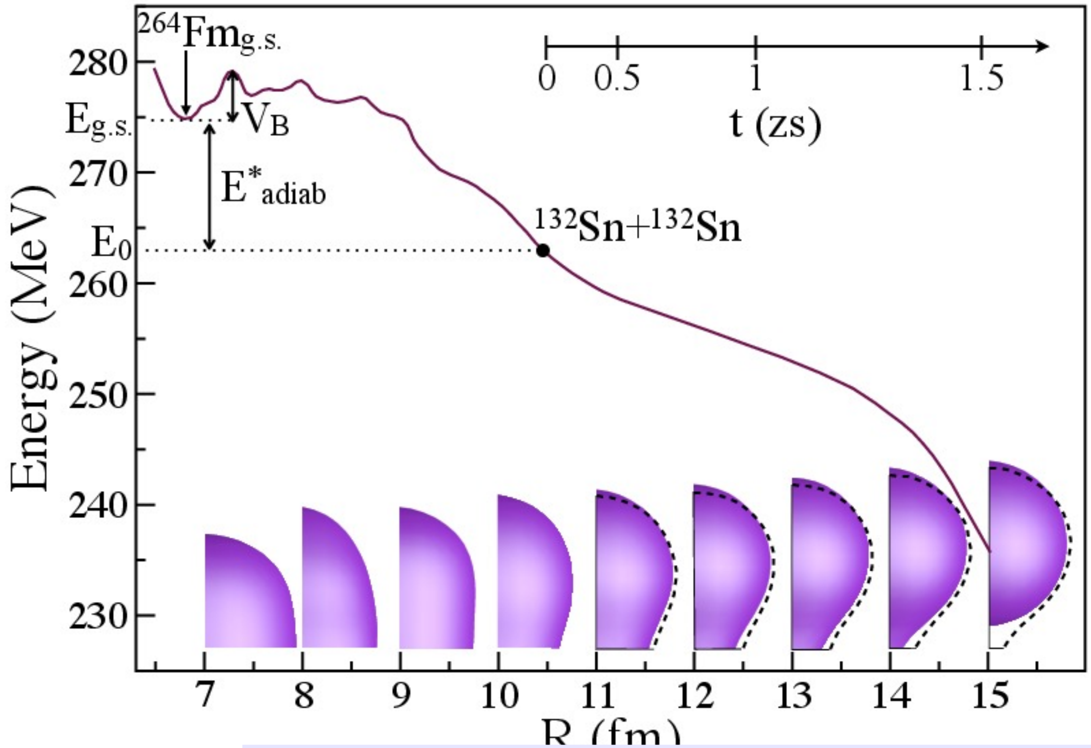


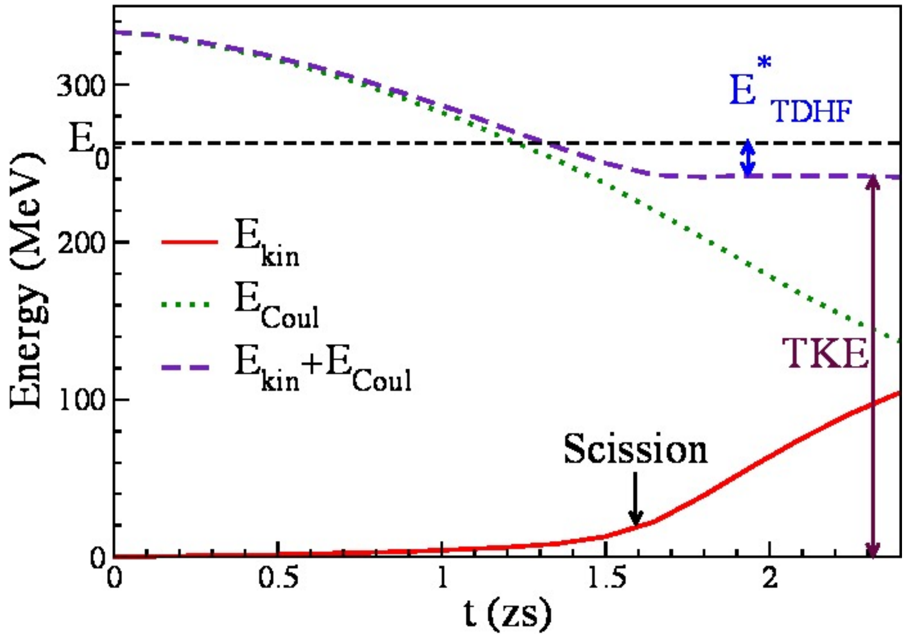
C. Simenel and A.S. Umar, PRC **89** (R), 031601 (2014)

J. Sadhukhan, K. Mazurek, A. Baran, J. Dobaczewski, W. Nazarewicz, and J. A. Sheikh, PRC **88**, 064314 (2013).

Scission Dynamics Using TDHF - Dynamics

- Start TDHF evolution at the point of fragment formation
- Compare results to adiabatic scission, can calculate TKE, E* etc.





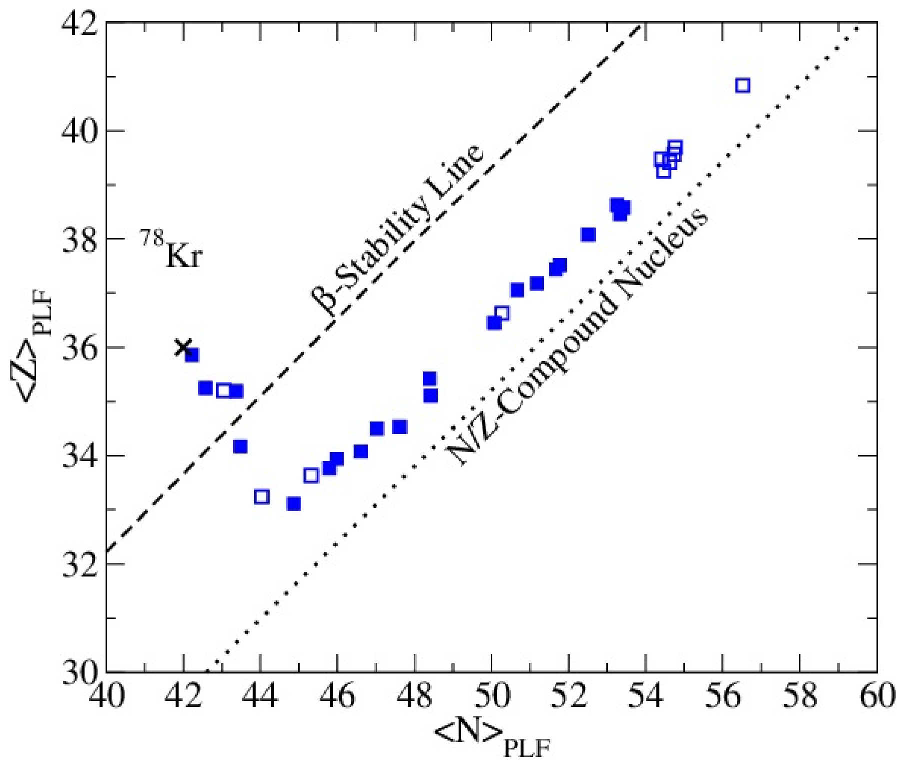
- Asymptotic TKE is around 241 MeV
- Adiabatic E* is about 12 MeV
- Dynamic TDHF E* is about 22 MeV leading to a total of 34 MeV excitation
- Also done 258Fm, TKE is 238-241 MeV (exp. Value 235 MeV).

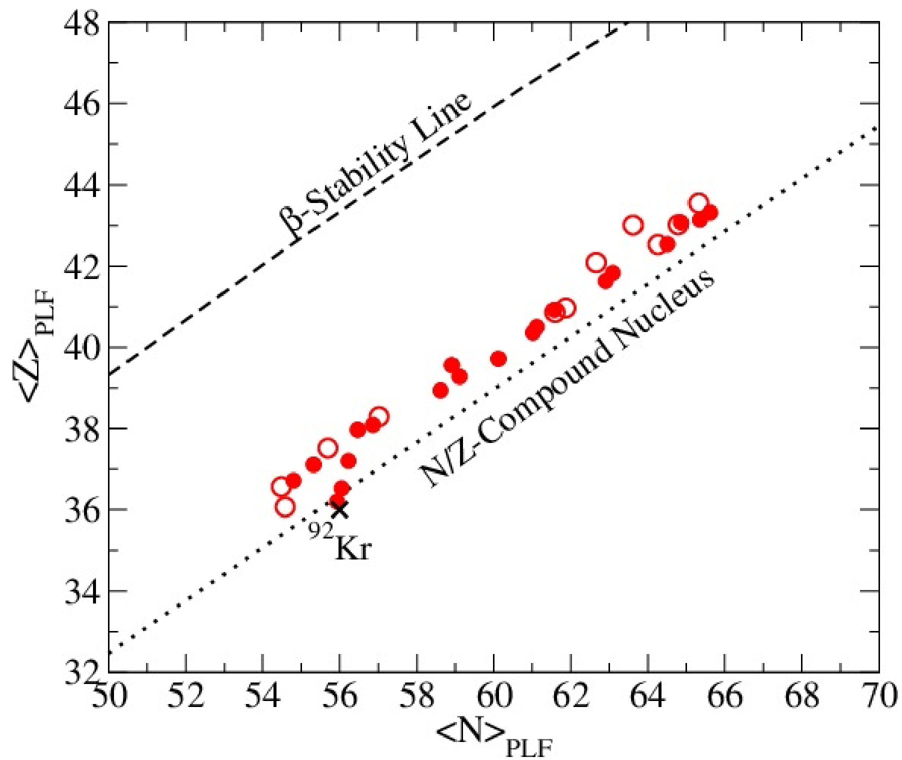
E.K. Hulet et al. **PRL** 56, 313 (1986)

Deep-Inelastic Collisions

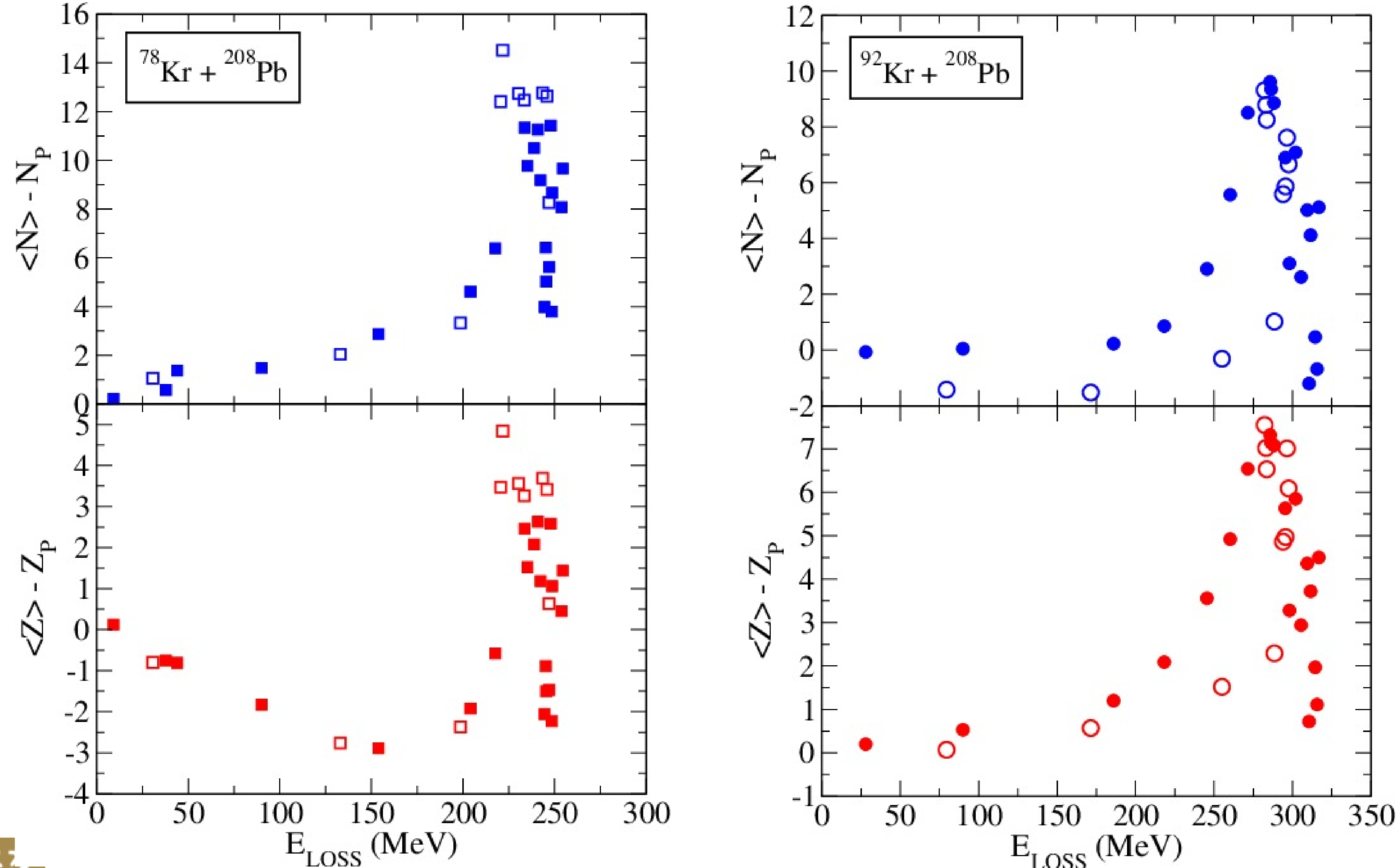
Deep-Inelastic Collisions – Isospin Transport

- SPIRAL2 experiment proposed for 78,92Kr+238U at E/A=8.5 MeV
- Transport properties with isospin asymmetric matter
- we have done calculations for 78,92Kr+208Pb at E/A=8.5 MeV
- Hollow points for β=90° orientation of 78,92Kr

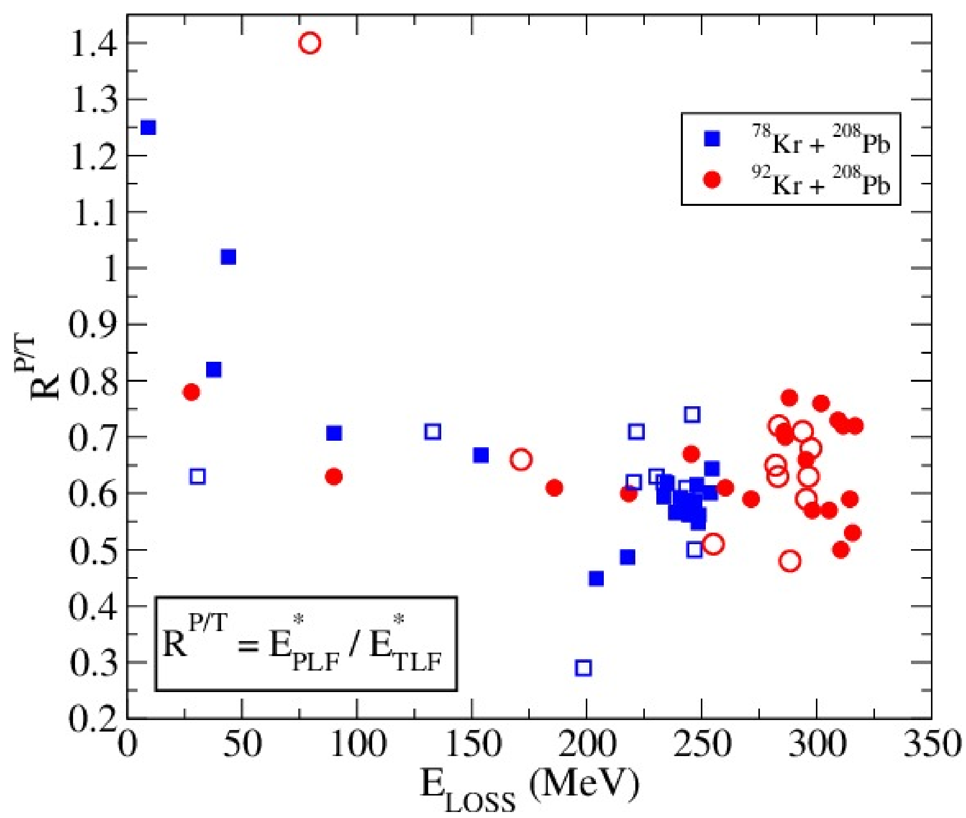


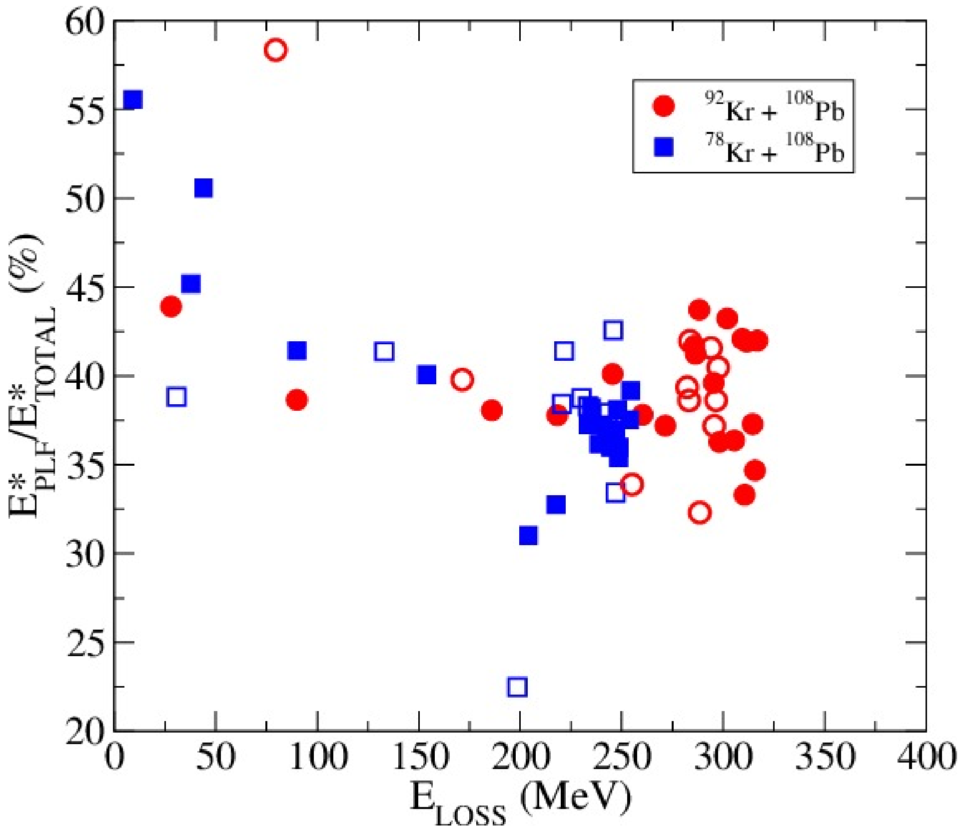


N_{PLF}, Z_{PLF} versus E_{LOSS}

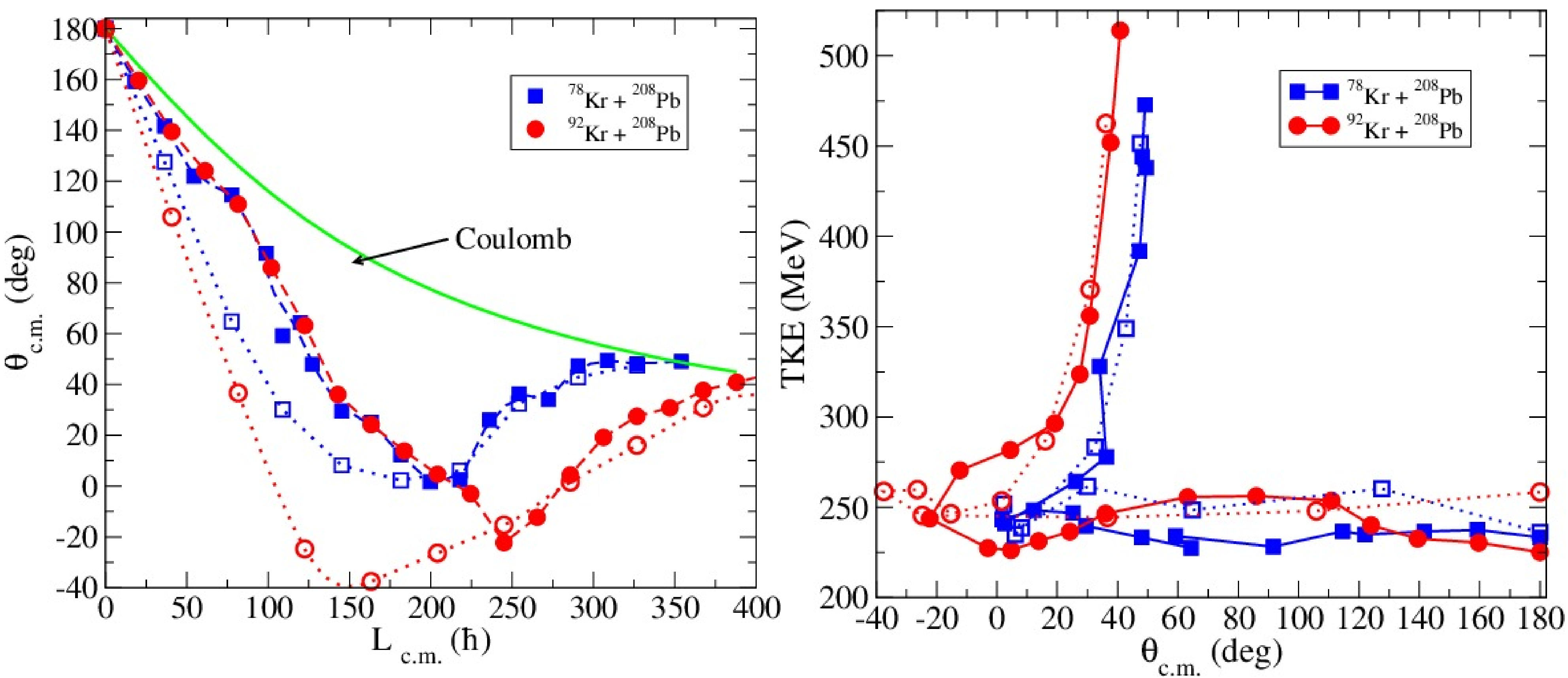


Sharing of Excitation Energy





Angular Properties of PLF



Summary

TDDFT have a strong place among the theories needed for future challenges of low-energy nuclear physics

Numerical issues are resolved – limitations only due to theoretical approximations (effective interactions, mean-field theory, etc.)

Quasifission and deep-inelastic reactions are well suited for TDDFT

We now have a reasonable handle on above- and sub-barrier fusion employing the DC-TDHF approach

One major and difficult area that needs attention is the dynamics of fission