Fusion and other applications of density-constrained TDDFT

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Outline of talk

standard TDHF: fusion above the barrier

DC-TDHF: fusion below and above the barrier

Observables:

fusion cross section $\sigma(E)$ for neutron-rich systems (RIB facilities)

average multi-nucleon transfer $\Delta N(R)$, $\Delta Z(R)$

pre-equilibrium excitation energy $E^*(R)$

pre-equilibrium GDR excitation and dipole spectrum dP/dE_γ

Capture cross sections for superheavy element formation

Fusion above the barrier: standard TDHF

Time-dependent Hartree-Fock (TDHF) theory

- Equations of motion obtained from variational principle

$$\delta S = \delta \int_{t_1}^{t_2} dt < \Phi(t) | H - i\hbar \frac{\partial}{\partial t} | \Phi(t) > = 0$$

- main approximation: many-body state is assumed to be a single time-dependent Slater determinant

$$\Phi(r_1, ..., r_A; t) = (A!)^{-1/2} \; det|\phi_\lambda(r_i, t)|$$

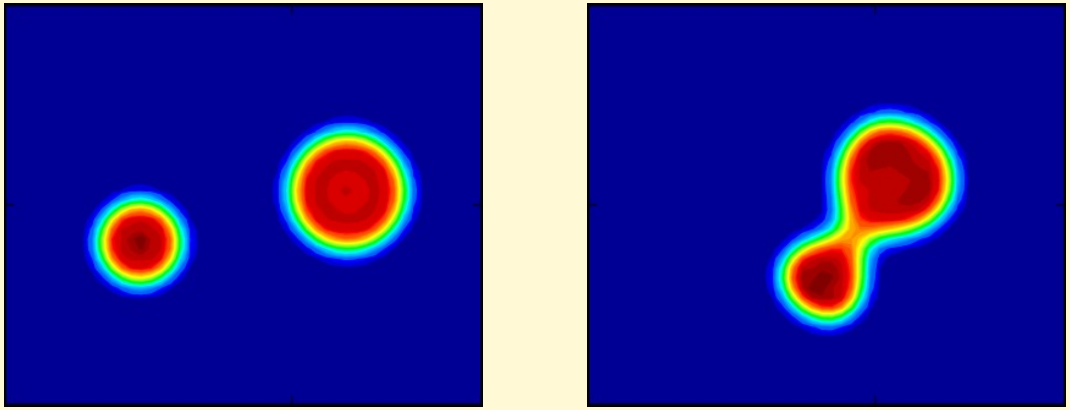
- TDHF equations for time-dependent single-particle states

$$h(\{\phi_\mu\}) \; \phi_\lambda(r,t) = i\hbar \frac{\partial}{\partial t} \phi_\lambda(r,t) \qquad (\lambda = 1, ..., A)$$

HF mean-field Hamiltonian $h = \partial E / \partial \rho$

A new generation TDHF Code: brief summary

A. S. Umar and V. E. Oberacker, PRC 73, 054607 (2006)

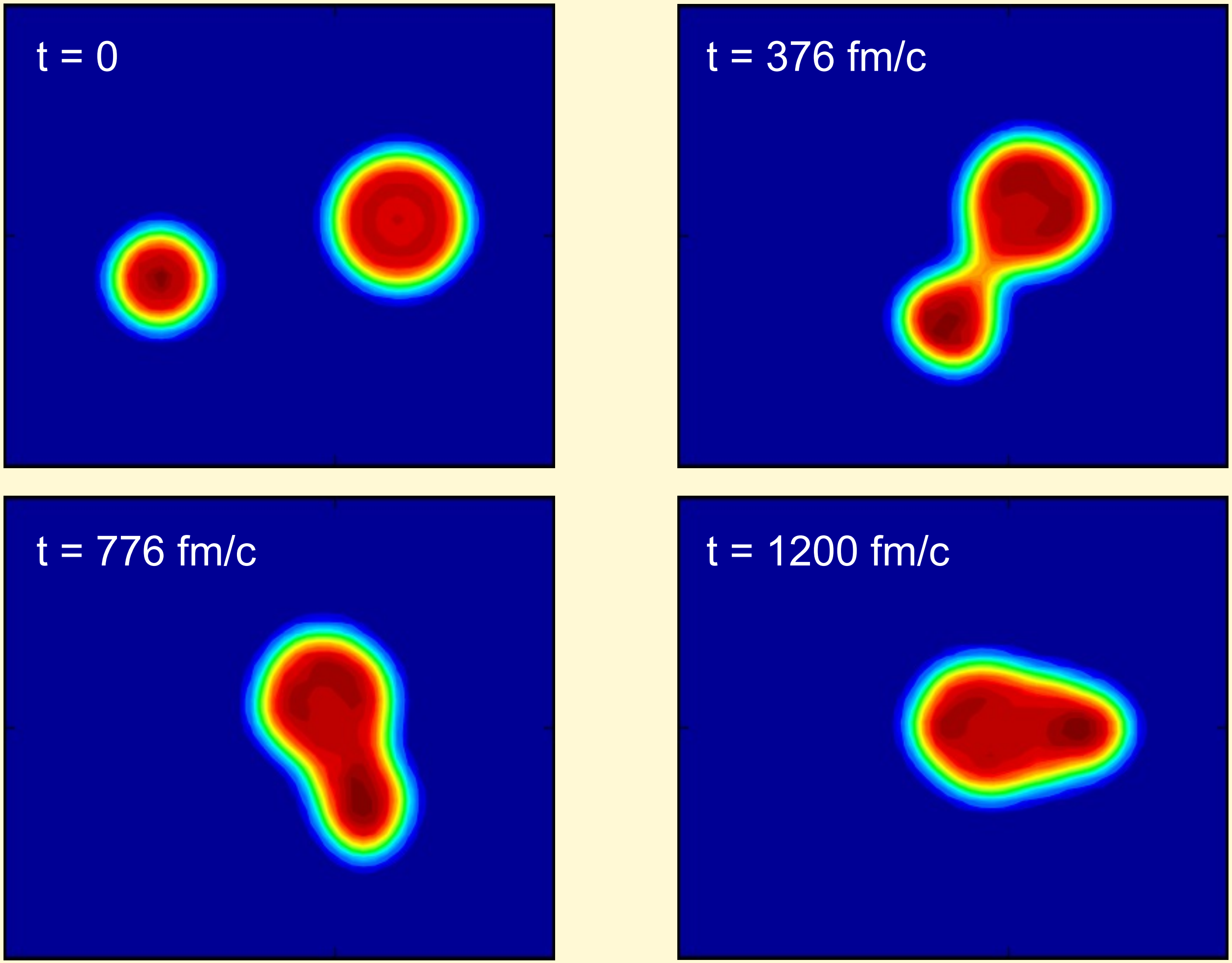


- 3-D Cartesian lattice
- Modern Skyrme forces with all terms (time-even /-odd)
- Coded in Fortran-95 and OpenMP
- Basis-Spline discretization for high accuracy

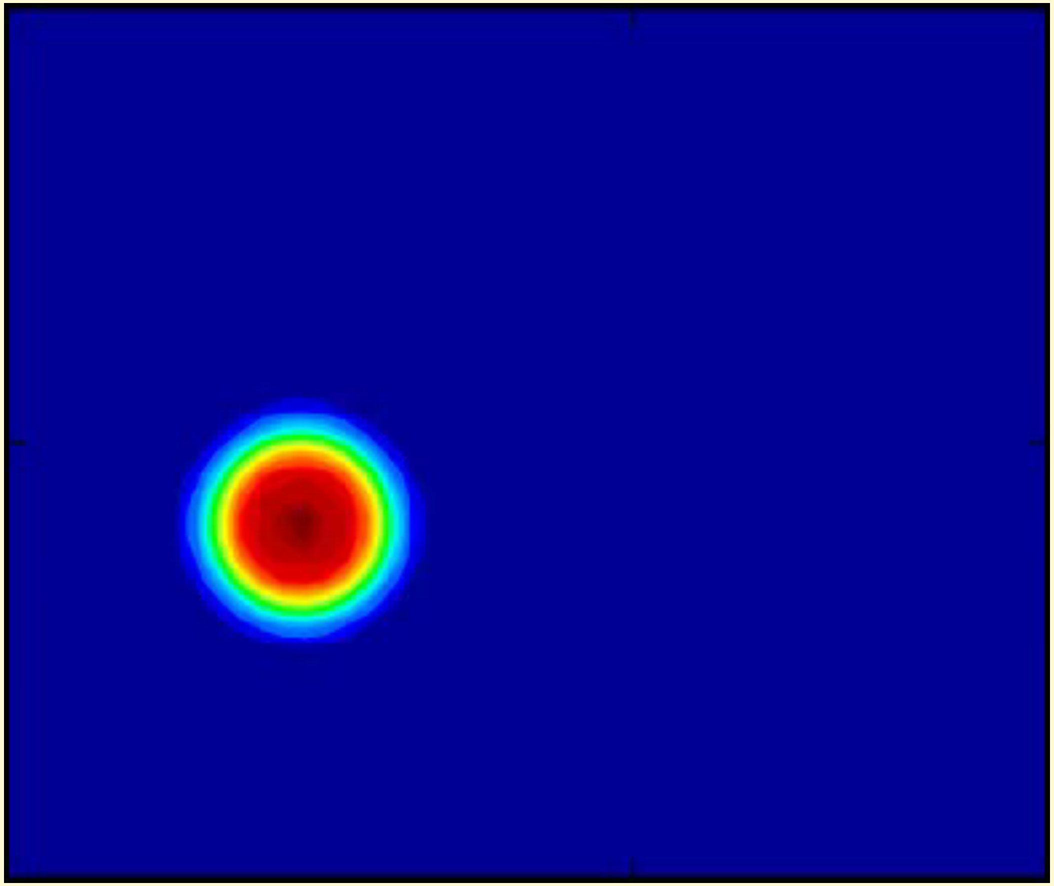
  Umar *et al.*, J. Comp. Phys. 93, 426 (1991)

$^{48}Ca + ^{132}Sn$, $E_{cm} = 130$ MeV, b = 4.45 fm (fusion)

TDHF, SLy4 interaction, 3-D lattice (50*40*30 points)

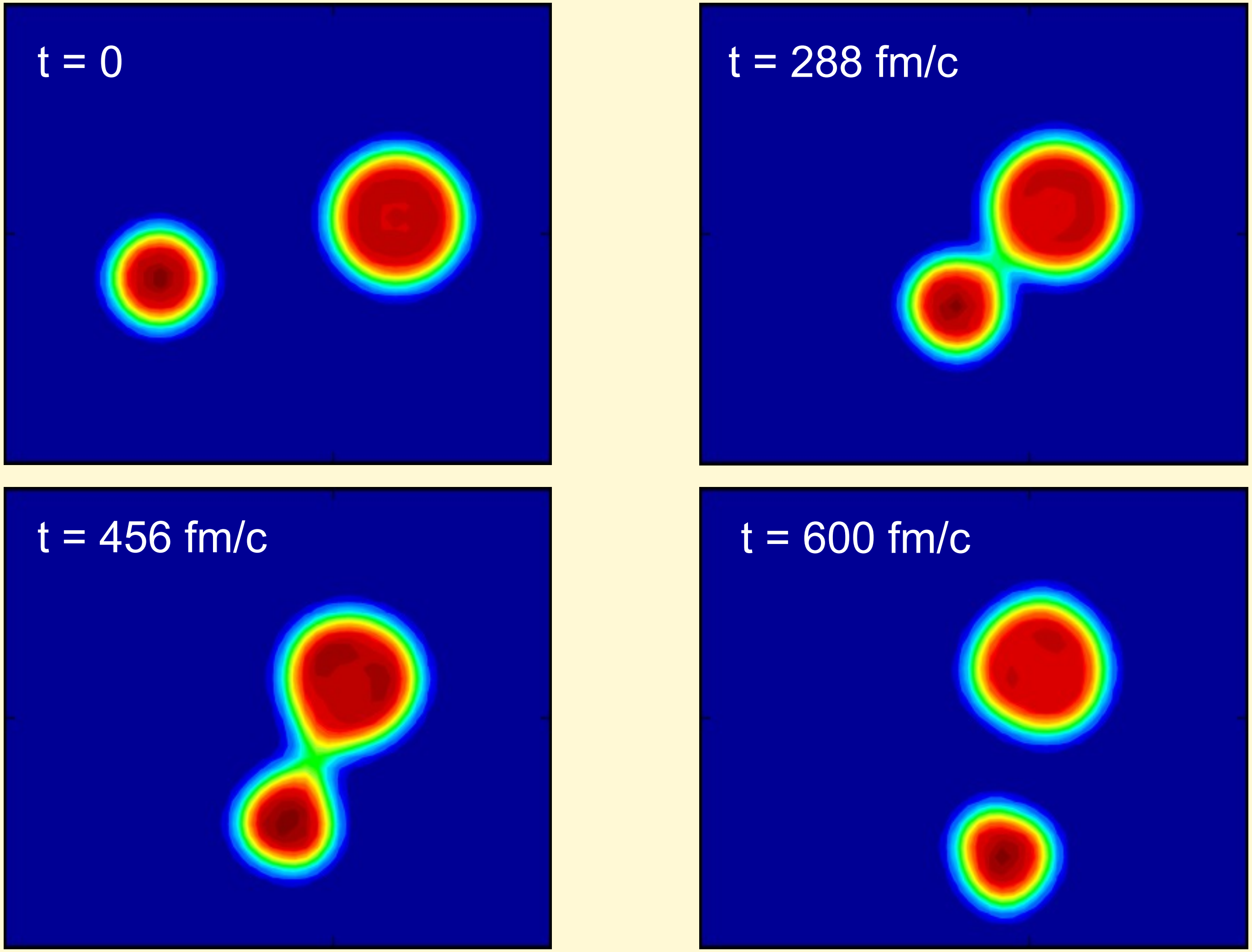


animation: ^{48}Ca+^{132}Sn, E_{cm} = 130 MeV, b = 4.45 fm (fusion)

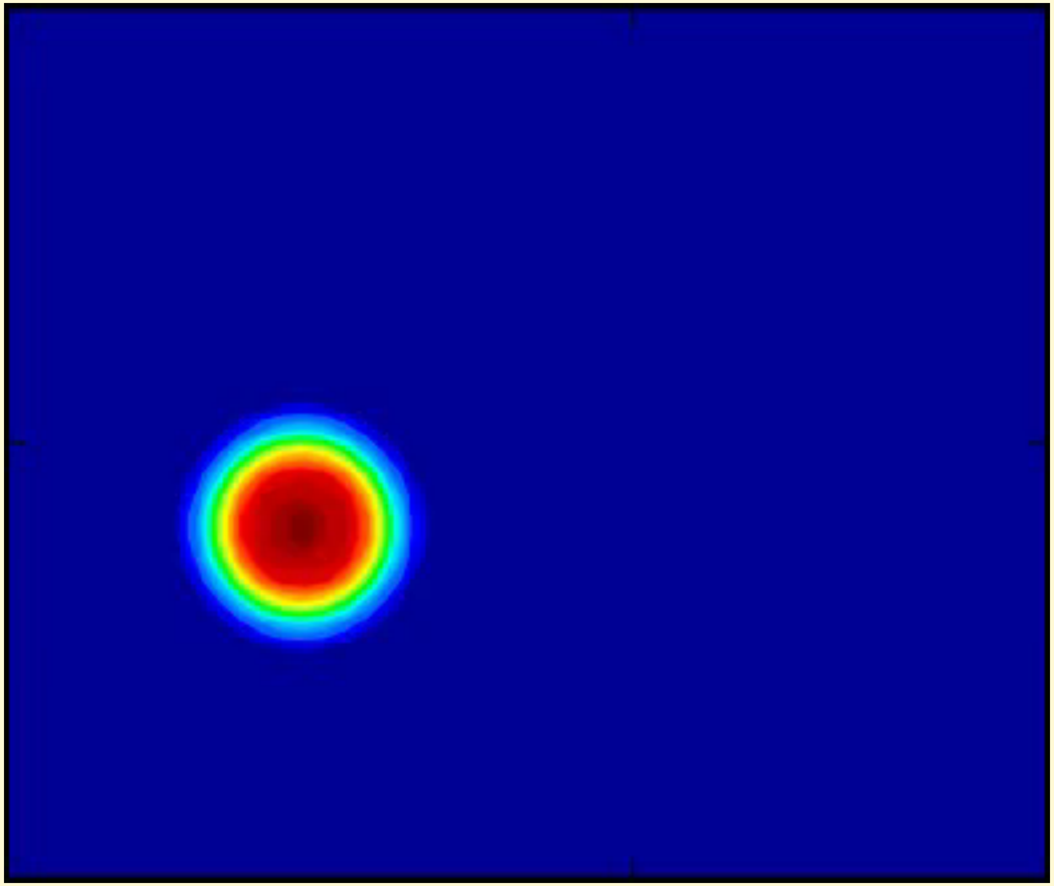


$^{48}Ca + ^{132}Sn$, E_{cm} = 130 MeV, b = 4.6 fm (deep-inelastic)

TDHF, SLy4 interaction, 3-D lattice (50*42*30 points)

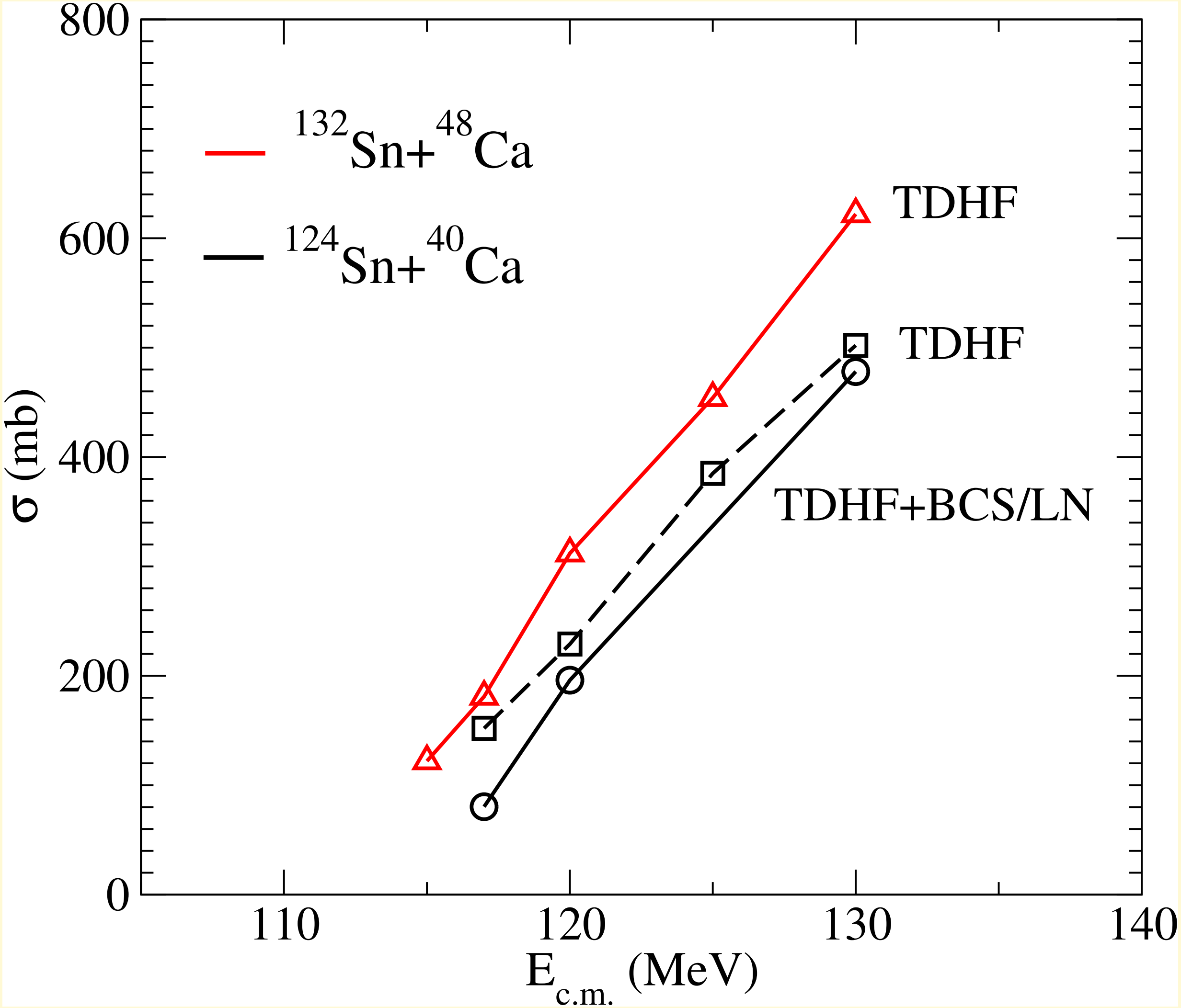


animation: $^{48}Ca+^{132}Sn$, E_{cm} = 130 MeV, b = 4.60 fm (deep-inel)



Fusion above the potential barrier (unrestricted TDHF)

Oberacker, Umar, Maruhn & Reinhard, Phys. Rev. C 85, 034609 (2012)



sharp cutoff model

$$\sigma_{fus} = \pi\ b^2_{max}$$

Fusion below and above the barrier: Density-Constrained TDHF (DC-TDHF)

Theoretical Description of Sub-Barrier Fusion

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

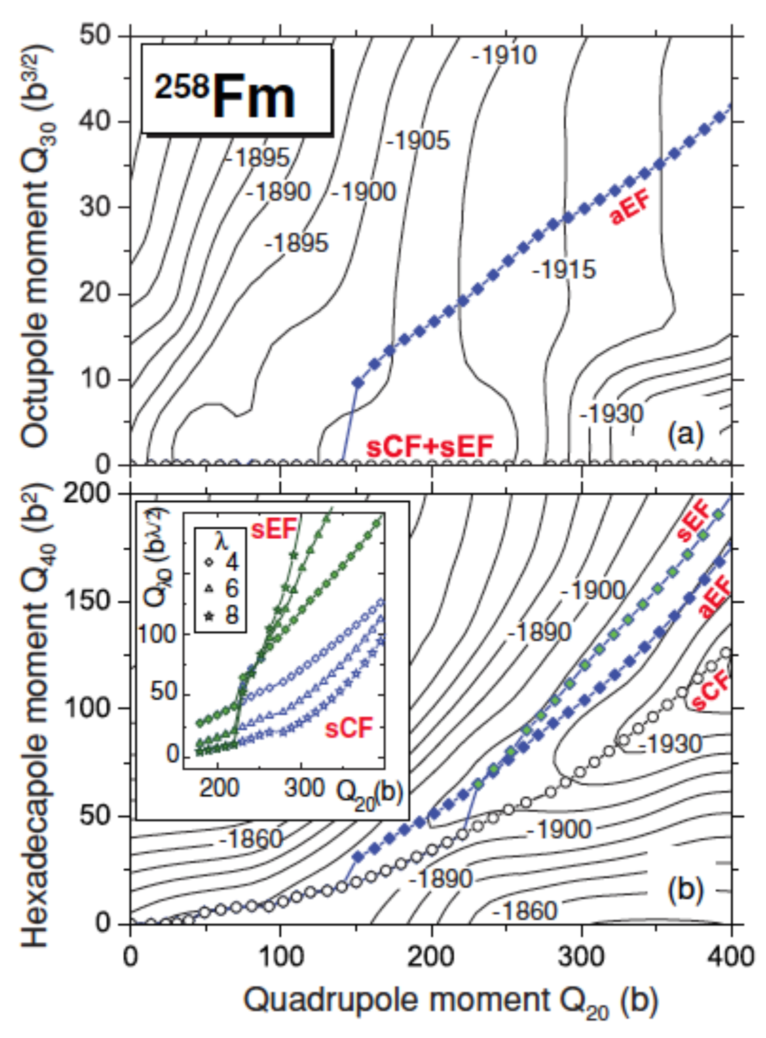
a) Calculate internuclear potential V(R)
- Woods-Saxon potential, proximity potential
  double-folding model with frozen densities (Esbensen)
- macroscopic-microscopic (Möller, Sierk)
- two-center shell model + liquid drop (Zagrebaev)
- microscopic: Skyrme + extended Thomas-Fermi (Wang, Scheid,…)
  constrained HF/HFB (Dobaczewski, Nazarewicz, …)
- our goal: time-dependent density functional theory, extract V(R)

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

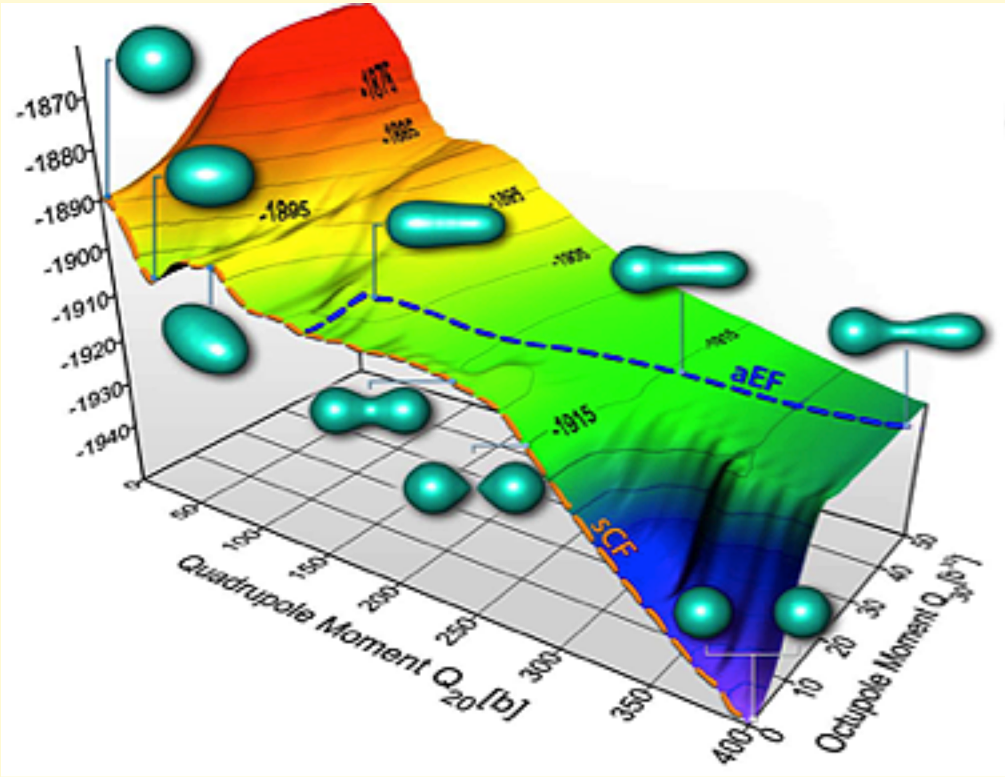
c) Incorporate inelastic and transfer channels
coupled channels approach (Esbensen, Hagino, …)

Brief review of standard constrained HF / HFB

$\delta < \Phi_0|H - \lambda_2 Q_{20} - \lambda_3 Q_{30}|\Phi_0 >= 0$ → potential energy surface $E(Q_{20},Q_{30})$



Staszczak, Baran, Dobaczewski & Nazarewicz, PRC 80, 014309 (2009)

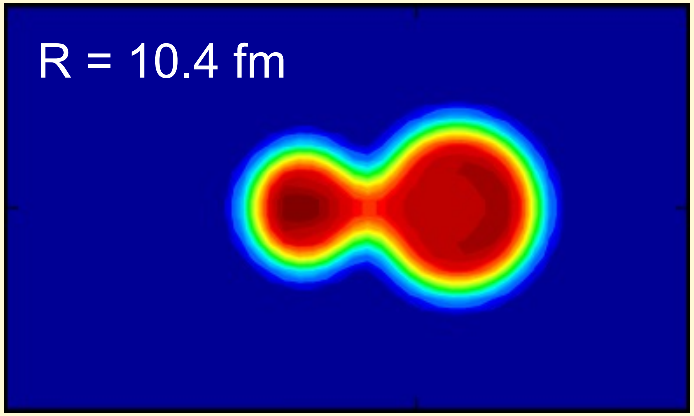


INT-13-3 Website

Density constrained TDHF (DC-TDHF): formalism

1. Run TDHF code at energy E_{cm} above potential barrier

2. Stop run at given internuclear distance R(t)



3. Take TDHF density

$$\rho_{\mathrm{TDHF}}(r,t) =< \Phi(t)|\rho|\Phi(t) >$$

and perform static HF energy minimization

$$\delta < \Phi_\rho \, |H - \int d^3r \; \lambda(r) \; \rho(r) \; |\Phi_\rho >= 0 \qquad \rightarrow |\Phi_\rho >$$

Lagrange multiplier

subject to density constraint $< \Phi_\rho|\rho|\Phi_\rho >= \rho_{\mathrm{TDHF}}(r,t)$

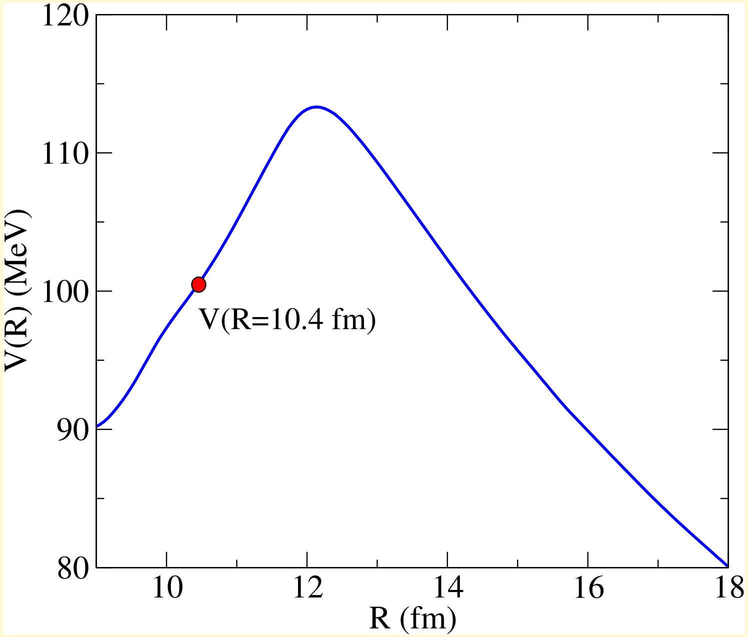
This takes out excitation energy E*(R).

4. Define density-constrained energy $E_{\mathrm{DC}}(R) =< \Phi_\rho|H|\Phi_\rho >$

DC-TDHF: calculate internuclear potential V(R)

Internuclear potential V(R) is equal to density-constrained energy $E_{DC}(R)$ minus binding energies of the two nuclei

$$V(R) = E_{\mathrm{DC}}(R) - E_{\mathrm{A}_1} - E_{\mathrm{A}_2}$$



DC-TDHF fusion calculations for $^{132,124}Sn + ^{48,40}Ca$

Detailed discussion of the following quantities:

internuclear potential $V(R)$

coordinate-dependent mass $M(R)$

fusion cross section $\sigma(E)$,

pre-equilibrium excitation energy $E^*(R)$

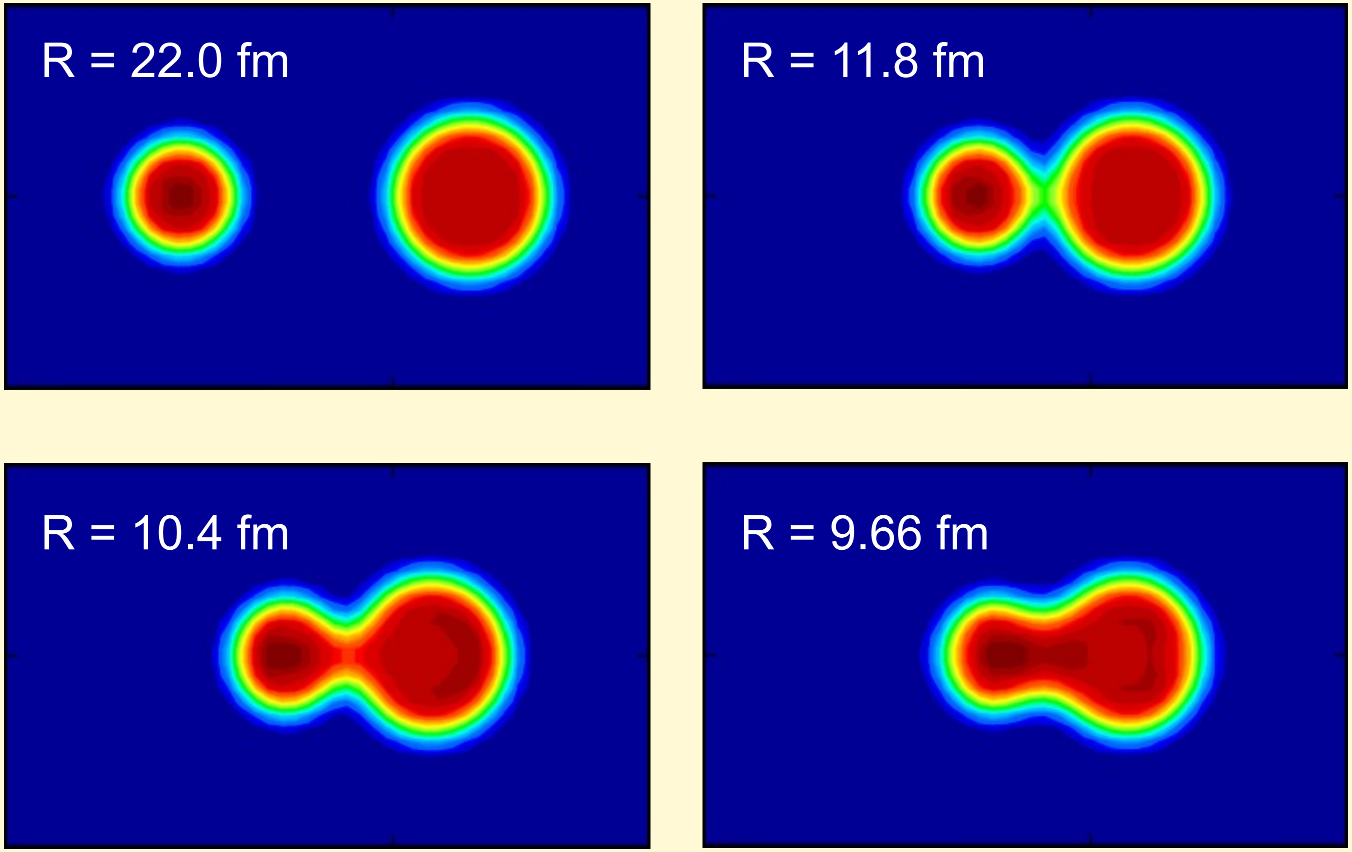
multi-nucleon transfer $\Delta N(R)$, $\Delta Z(R)$

pre-equilibrium GDR excitation and dipole spectrum dP/dE_γ

Calculation of internuclear potential with DC-TDHF method

$$V(R) = E_{\mathrm{DC}}(R) - E_{\mathrm{A}_1} - E_{\mathrm{A}_2}$$

Oberacker, Umar & Keser, NN2012 conference, J. Phys. Conf. Series 420 (2013) 012132

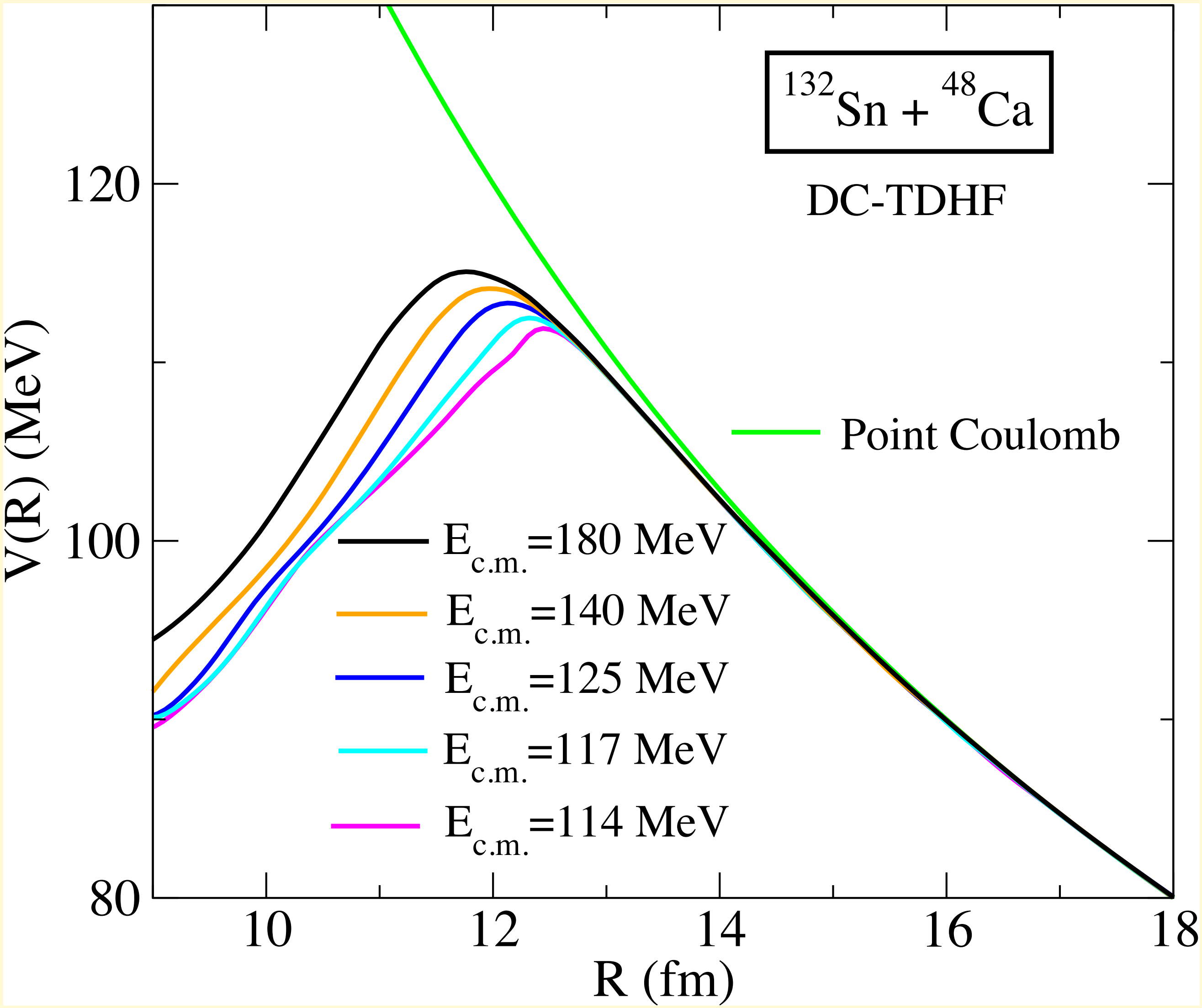


$^{48}Ca+^{132}Sn$
E_{cm}=140 MeV

V(R) contains dynamical entrance channel effects (neck formation, particle transfer, surface vibrations, giant resonances)

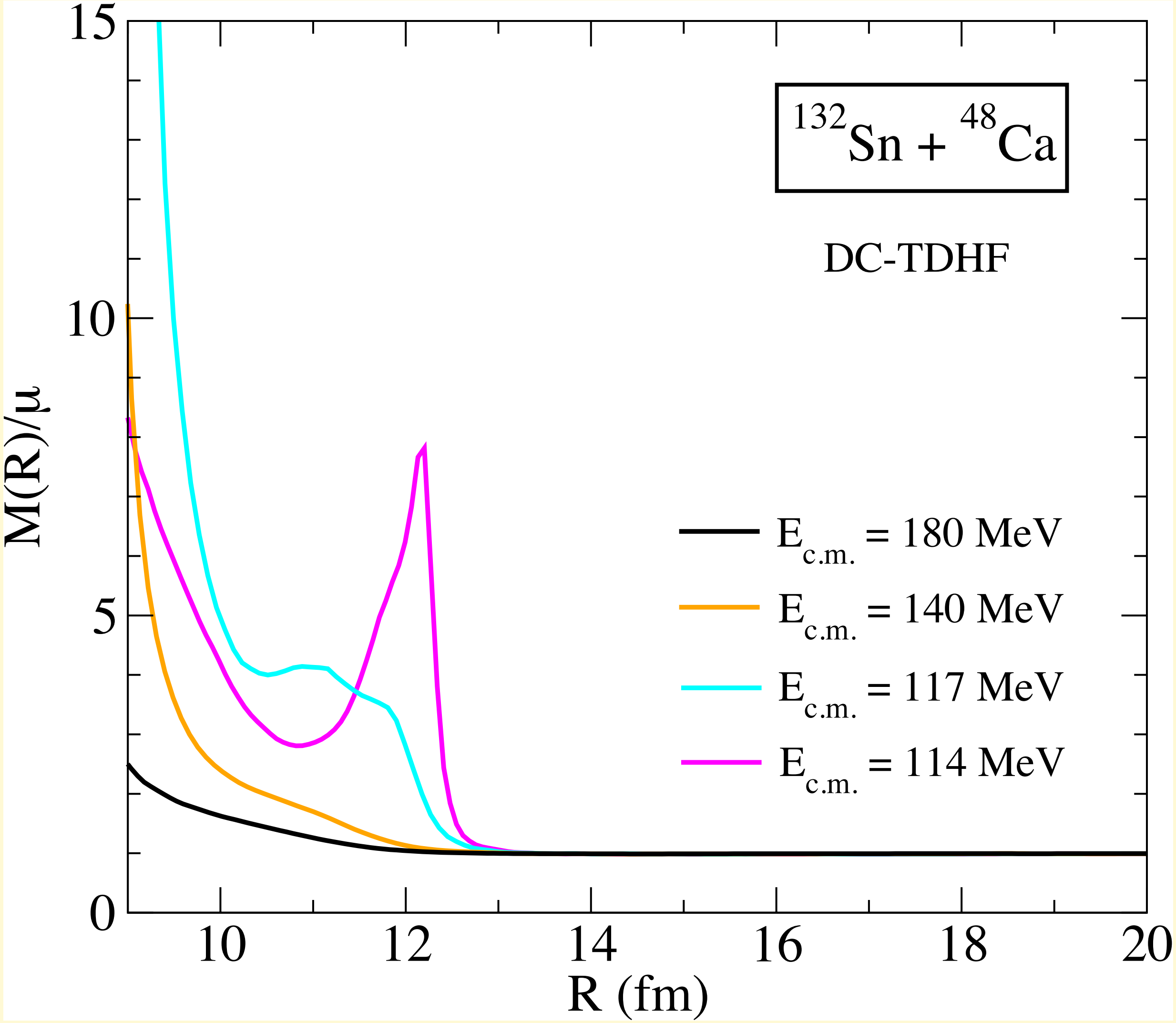
Internuclear potential: strong E_{cm}-dependence

Oberacker, Umar, Maruhn & Reinhard, Phys. Rev. C 85, 034609 (2012)



Mass parameter: strong E_{cm}-dependence

Oberacker, Umar, Maruhn & Reinhard, Phys. Rev. C 85, 034609 (2012)



Scale transformation to constant reduced mass μ

Umar & Oberacker, Eur. Phys. J. A 39, 243 (2009)

$$\frac{1}{2}M(R)(\frac{dR}{dt})^2 = \frac{1}{2}\mu(\frac{d\bar{R}}{dt})^2 \qquad d\bar{R} = \left(\frac{M(R)}{\mu}\right)^{\frac{1}{2}} dR$$

scaled distance

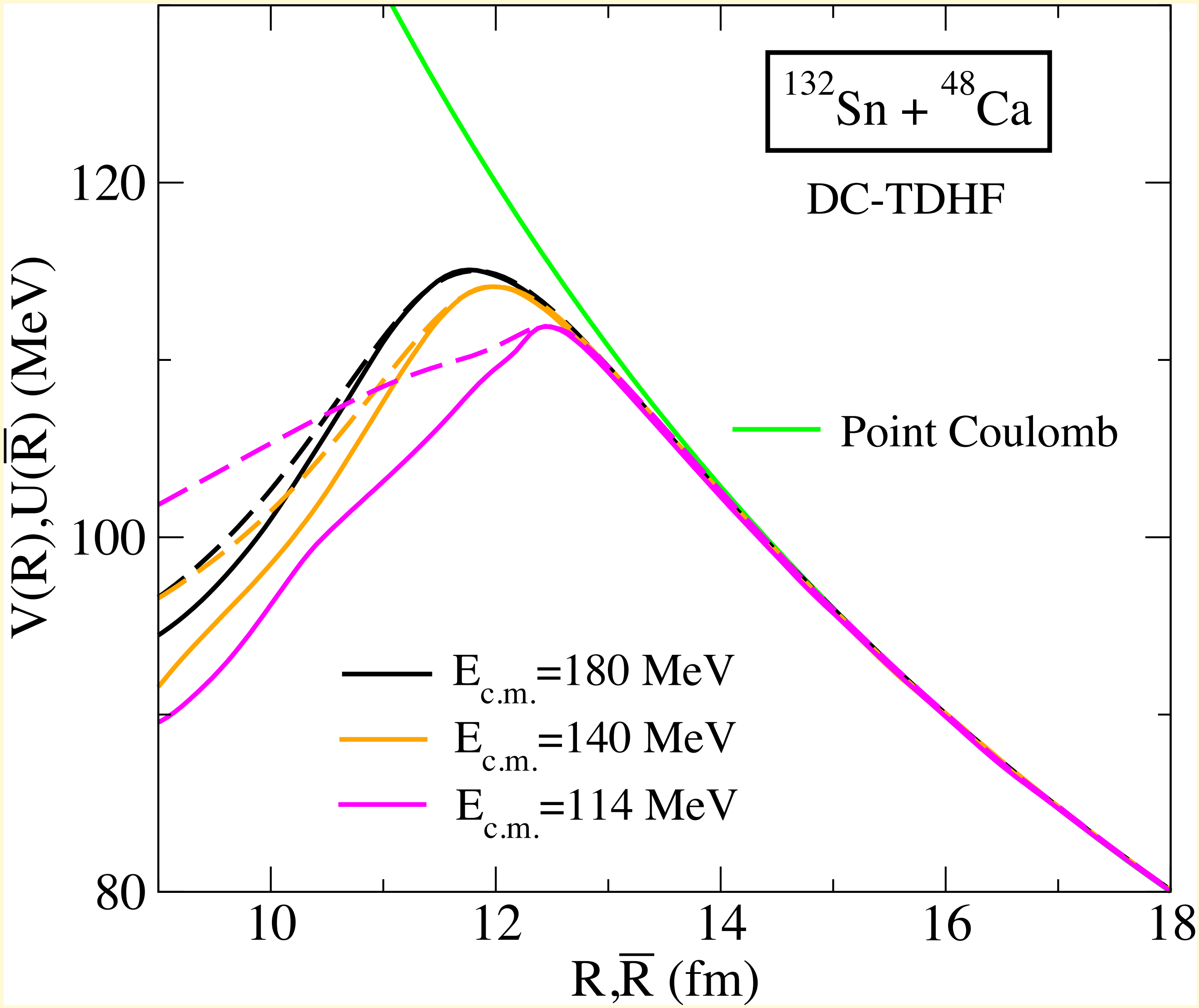
integrate $\quad \bar{R} = f(R) \quad \Longleftrightarrow \quad R = f^{-1}(\bar{R})$

$$V(R) = V(f^{-1}(\bar{R})) = U(\bar{R})$$

original potential transformed potential

Transformed internuclear potential

Oberacker, Umar, Maruhn & Reinhard, Phys. Rev. C 85, 034609 (2012)



Total fusion cross section for two spherical nuclei

$$\sigma_{\text{fus}}(E_{\text{c.m.}}) = \frac{\pi\hbar^2}{2\mu E_{\text{c.m.}}} \sum_{\ell=0}^{\infty} (2\ell+1) T_\ell(E_{\text{c.m.}})$$

Schrödinger equation for transformed radial coordinate

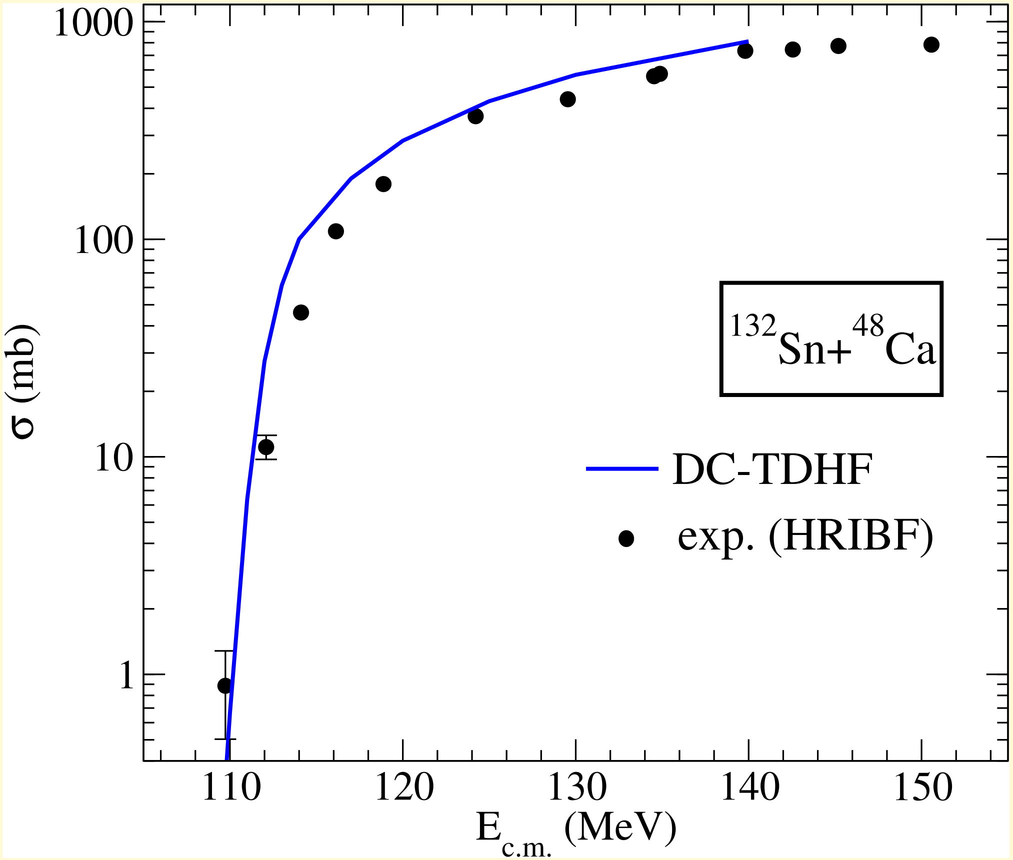
$$\left[\frac{-\hbar^2}{2\mu} \frac{d^2}{d\bar{R}^2} + \frac{\hbar^2 \ell(\ell+1)}{2\mu \bar{R}^2} + U(\bar{R}) - E_{\text{c.m.}} \right] \psi_\ell(\bar{R}) = 0$$

reduced mass

transformed potential

solve Schrödinger equation numerically, with Incoming Wave Boundary Condition (IWBC) $\rightarrow T_\ell(E_{\text{c.m.}})$

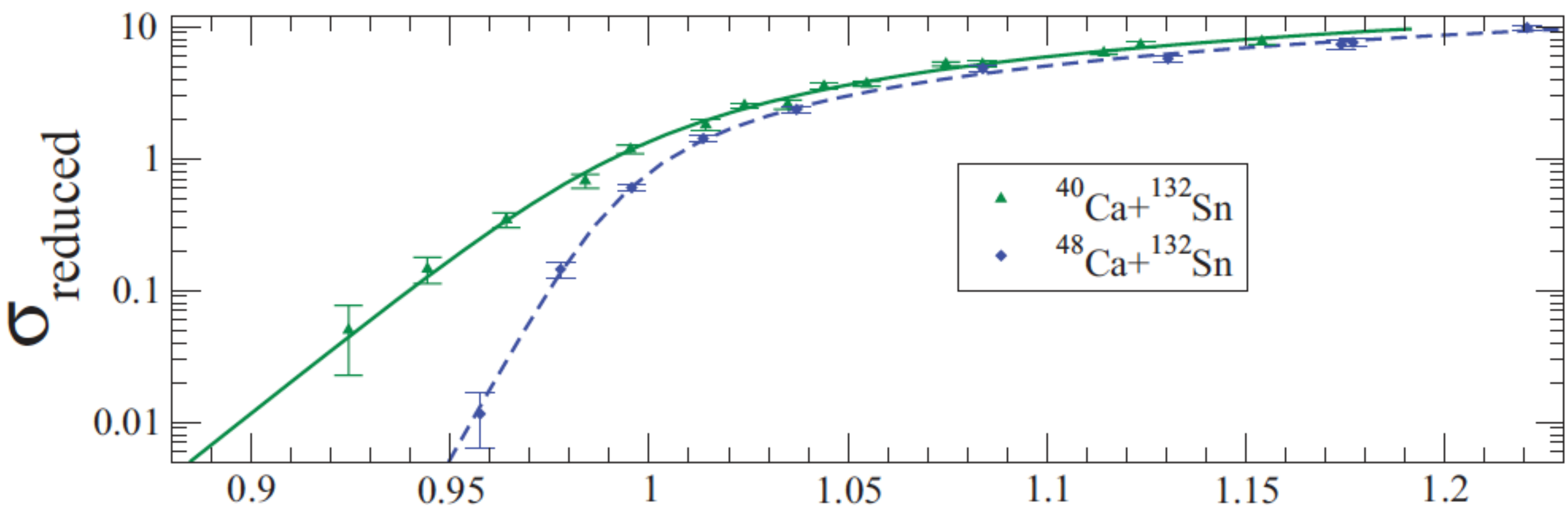
Theory: Oberacker, Umar, Maruhn & Reinhard, PRC 85, 034609 (2012)
Oberacker & Umar, PRC 87, 034611 (2013)



exp. data (HRIBF): J.J. Kolata, A. Roberts, A.M. Howard, D. Shapira, J.F. Liang, C.J. Gross, R.L. Varner, Z. Kohley, A.N. Villano, H. Amro, W. Loveland, and E. Chavez, Phys. Rev. C 85, 054603 (2012)

Anomaly in sub-barrier fusion cross sections for $^{132}Sn+^{40,48}Ca$

Q_{gg} (^{40}Ca fusion) = -52.1 MeV, Q_{gg} (^{48}Ca fusion) = -76.2 MeV

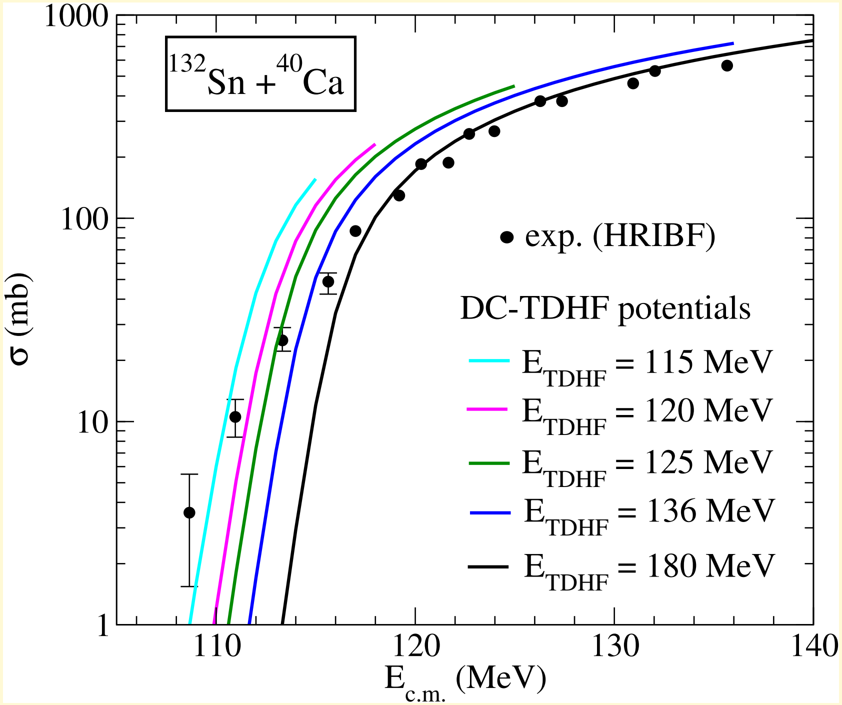


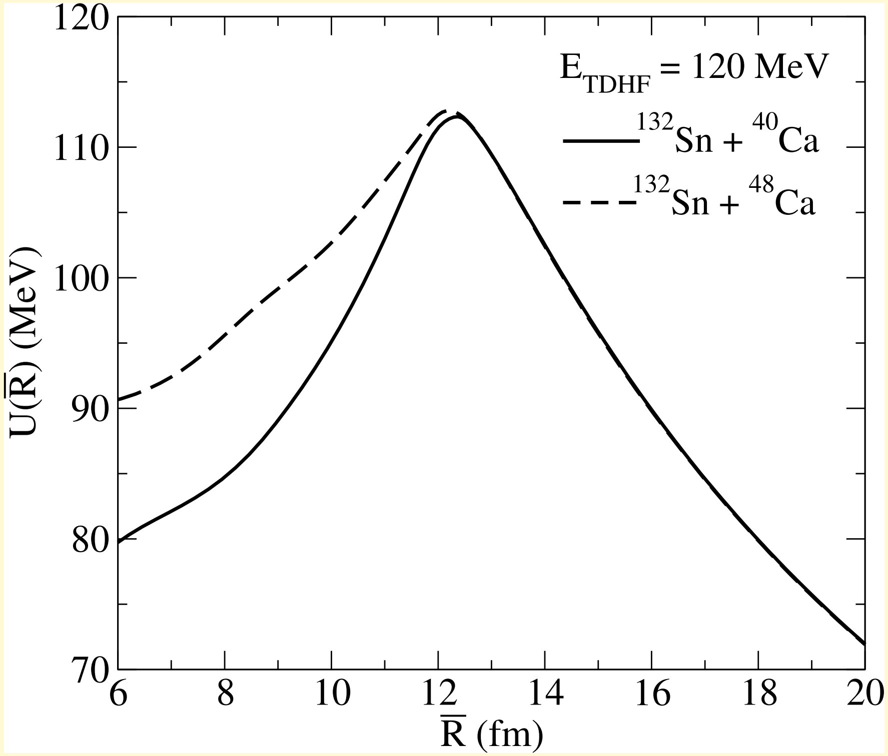
exp. data (HRIBF): J.J. Kolata, A. Roberts, A.M. Howard, D. Shapira, J.F. Liang, C.J. Gross, R.L. Varner, Z. Kohley, A.N. Villano, H. Amro, W. Loveland, and E. Chavez, Phys. Rev. C 85, 054603 (2012)

Explanation of fusion anomaly in ^{132}Sn+^{40,48}Ca

The width of the DC-TDHF potential barrier for ^{40}Ca is substantially smaller than for ^{48}Ca, resulting in enhanced sub-barrier fusion

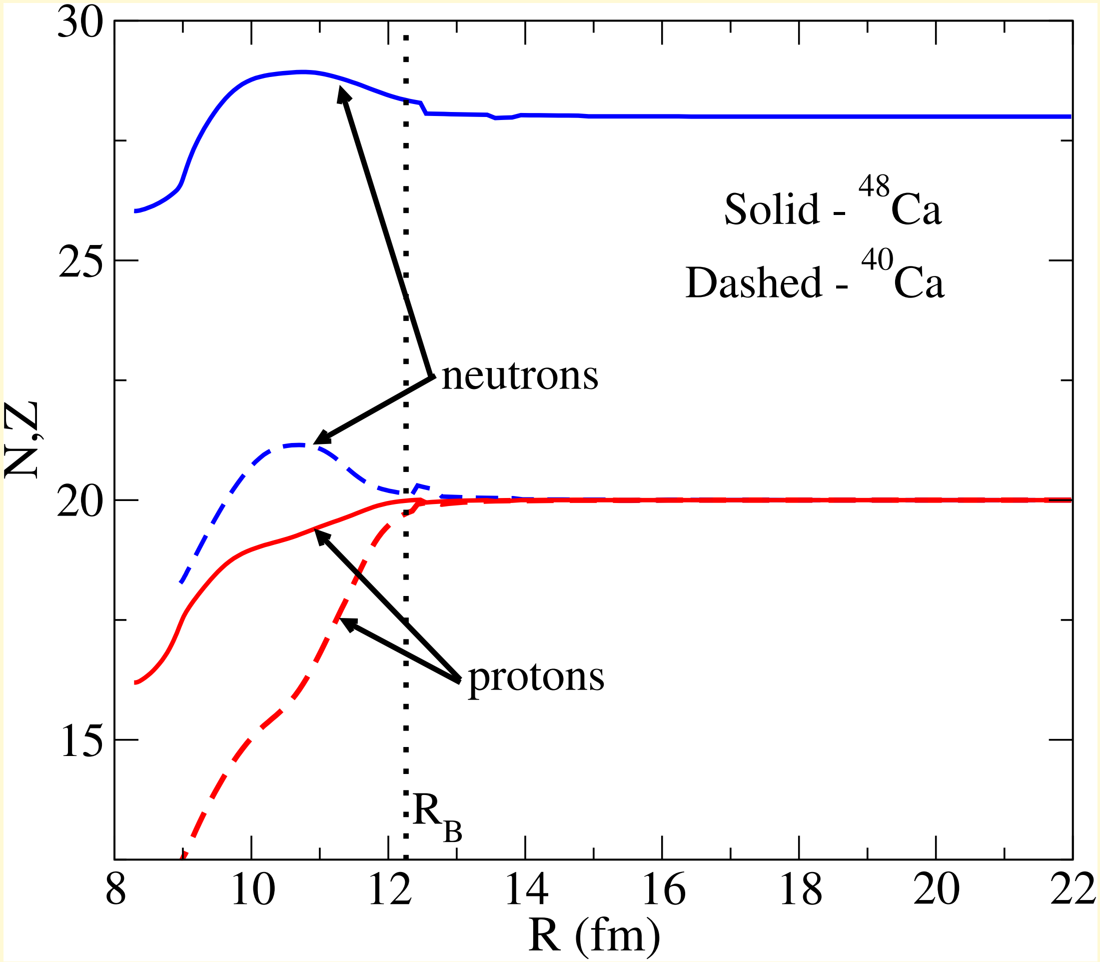
Ref: Oberacker & Umar, PRC 87, 034611 (2013)





Multi-nucleon transfer in $^{132}Sn+^{40,48}Ca$

Ref: Oberacker & Umar, PRC 87, 034611 (2013)



E_{cm}=120 MeV, b=0

$^{132}Sn+^{40}Ca$
Q (n-pickup) > 0
Q (p-stripping) > 0

$^{132}Sn+^{48}Ca$
Q (n-pickup) < 0
Q (p-stripping) < 0

Dynamic excitation energy E*(R(t))

Ref: Umar, Oberacker, Maruhn & and Reinhard, PRC 80, 041601(R) (2009)

collective energy $E_{coll}(t) = E_{kin}(\rho(t), j(t)) + E_{DC}(\rho(t))$

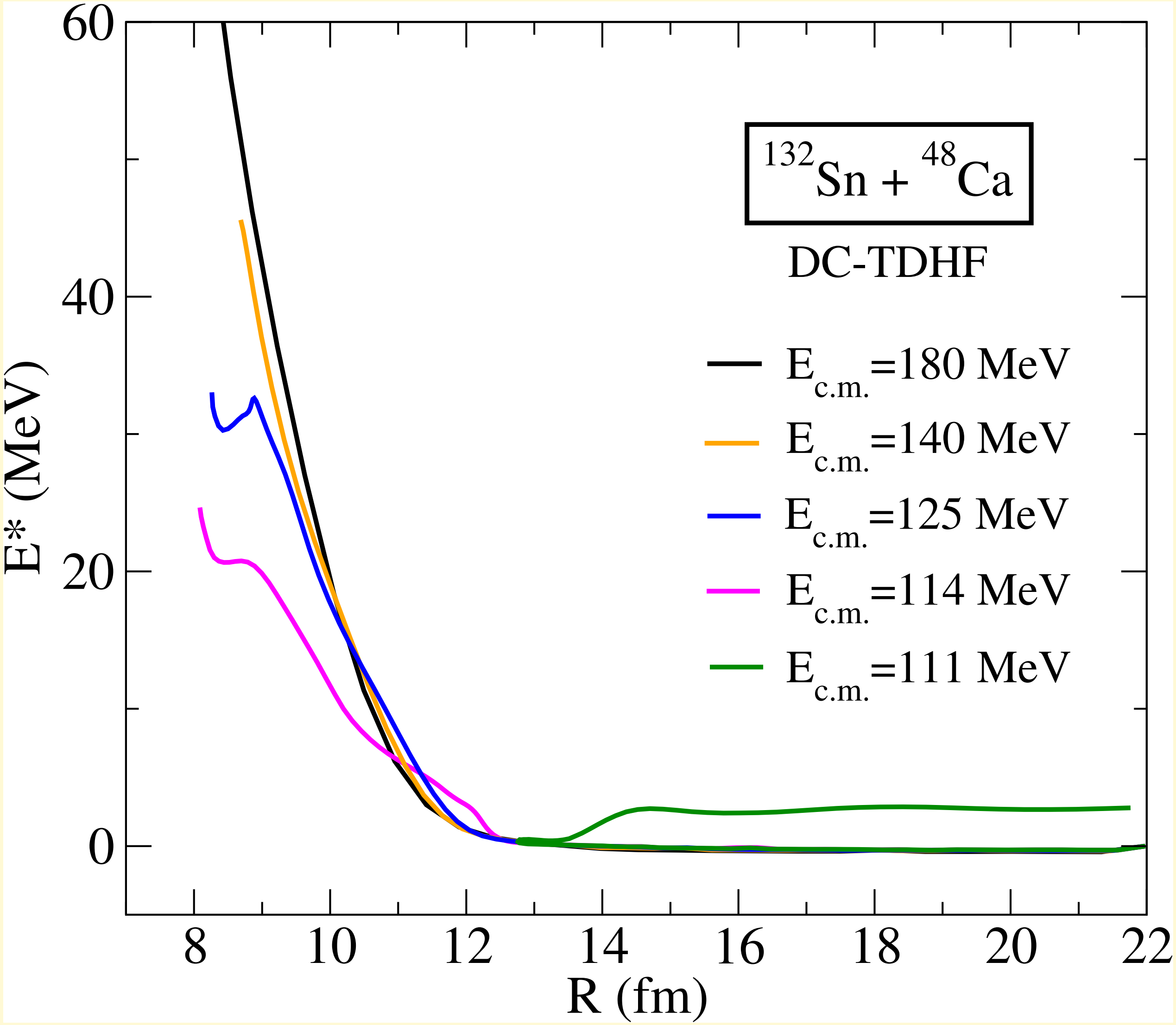
excitation energy $E^*(R(t)) = E_{TDHF} - E_{coll}(t)$

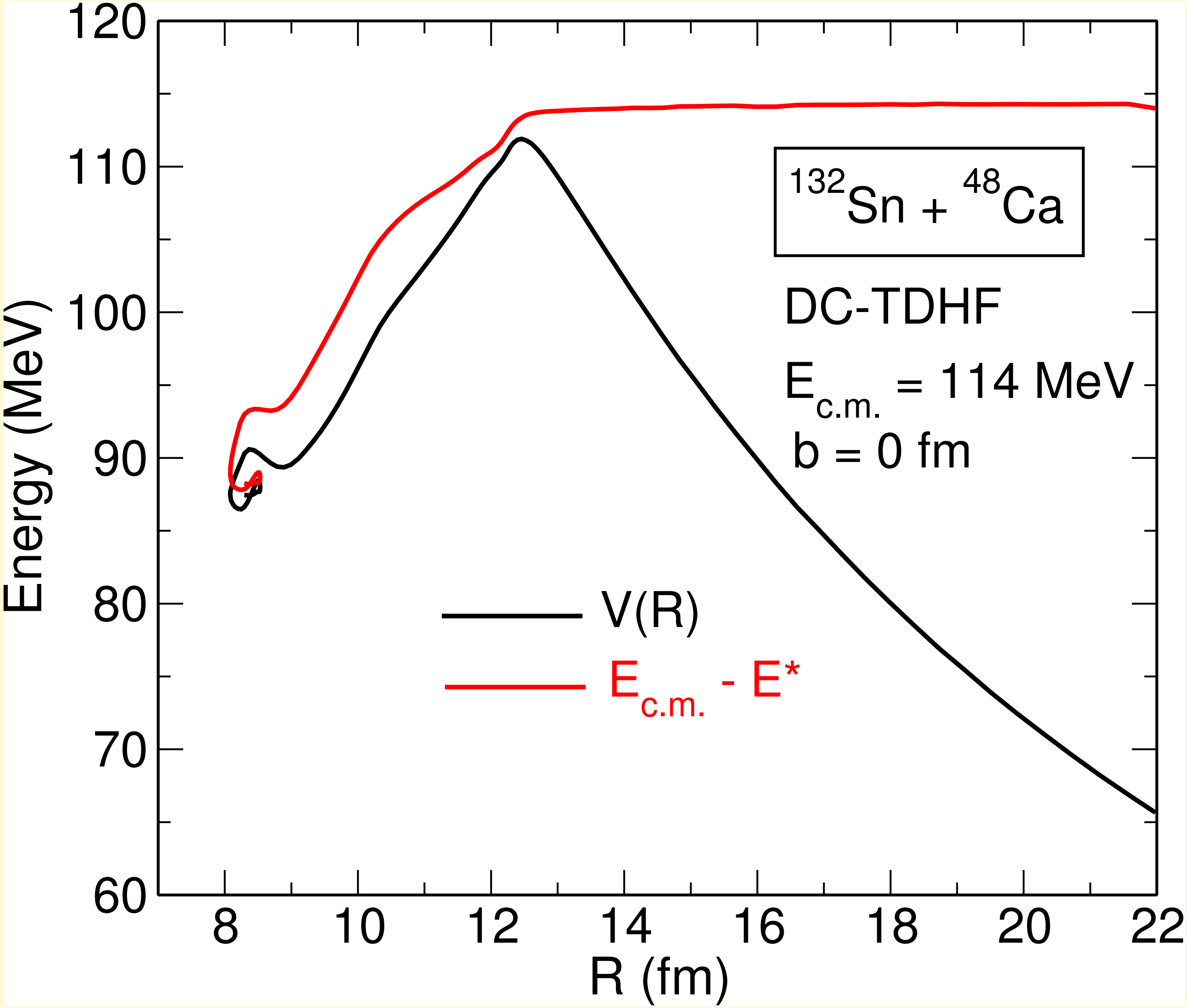
$$E^*(R(t)) = E_{TDHF} - E_{kin}((t)) - E_{DC}((t))$$

Approximate expression for collective kinetic energy

$$E_{kin}(\rho(t), j(t)) \approx \frac{m}{2} \int d^3r \frac{j^2(t)}{\rho(t)} \xrightarrow[\text{large R}]{} \frac{\mu}{2}\dot{R}^2$$

Dynamic excitation energy E*(R(t))





132Sn + 48Ca
DC-TDHF
E c.m. = 114 MeV
b = 0 fm
V(R)
E c.m. - E*
Energy (MeV)
R (fm)
120
110
100
90
80
70
60
8
10
12
14
16
18
20
22

Pre-equilibrium GDR excitation and dipole radiation in heavy-ion fusion reactions

Goal: info about early stages of heavy-ion fusion reaction, elongated shape (β_2=0.6) during pre-equilibrium phase.

Unrestricted TDHF: $^{132}Sn+^{48}Ca$ (E_{cm} =130 MeV, b=0 fm)

Compare to $^{124}Sn+^{40}Ca$

Study dynamical density oscillations as function of time

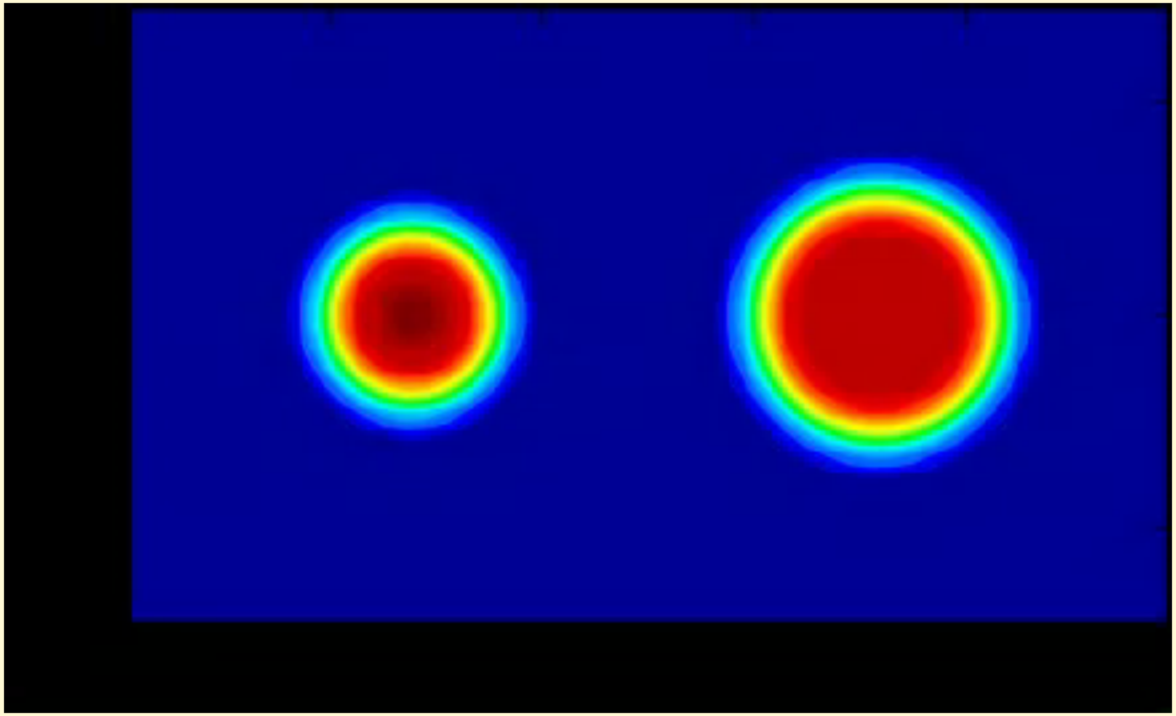
Compute dynamical dipole moment D(t) and EM radiation

- Umar & Oberacker, PRC 76, 014614 (2007)
- Simenel, Chomaz & de France, PRC 76, 024609 (2007)
- Baran, Rizzo, Colonna, Di Toro & Pierroutsakou, PRC 79, 021603(R) (2009)
- Oberacker, Umar, Maruhn & Reinhard, PRC 85, 034609 (2012)
- Keser, Umar & Oberacker, PRC 85, 044606 (2012)

Animation: dynamic giant resonance excitation:

$^{48}Ca + ^{132}Sn$, $E_{cm} = 130$ MeV, $b = 0$ (fusion)

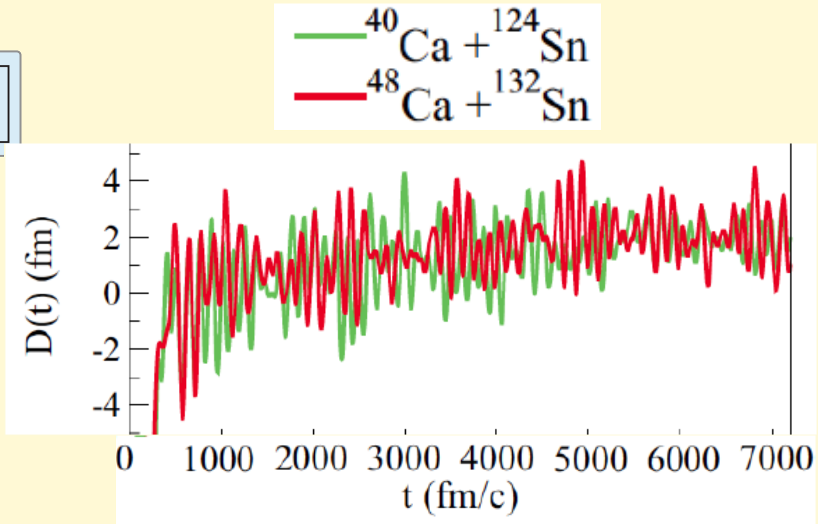
TDHF, SLy4 interaction, $t_{final} = 7{,}200$ fm/c



Pre-equilibrium GDR Excitation

dipole moment as a function of time (TDHF)

$$D(t) = \frac{NZ}{A}\left[\frac{1}{Z}\sum_{p=1}^{Z} < x_p(t) > - \frac{1}{N}\sum_{n=1}^{N} < x_n(t) >\right]$$



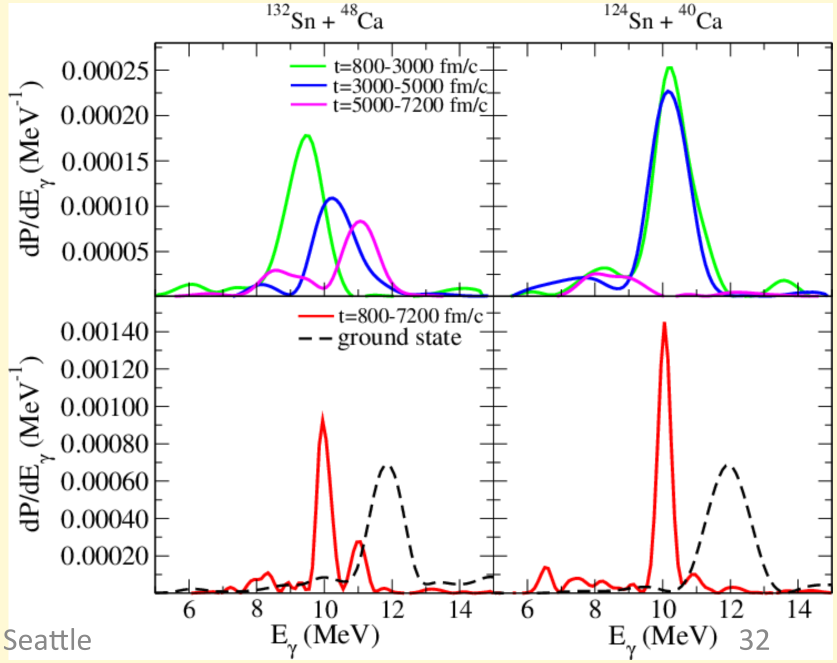
Power spectrum of electric dipole radiation

$$\frac{dP}{dE_\gamma} = \frac{2\alpha}{3\pi E_\gamma}\left|\frac{1}{c}D''(\omega)\right|^2$$

$$\alpha = e^2/(\hbar c) \approx 1/137$$

Pre-equilibrium GDR is stronger for systems with larger initial N/Z differential of the two ions:

1.48 : 1.0 for ^{124}Sn+^{40}Ca,
1.64 : 1.4 for ^{132}Sn+^{48}Ca



Ref: Oberacker, Umar, Maruhn & Reinhard, PRC 85, 034609 (2012)

DC-TDHF fusion calculations
for other systems

(about 25 fusion reactions
studied between 2006-2013)

DC-TDHF fusion calculations for light systems

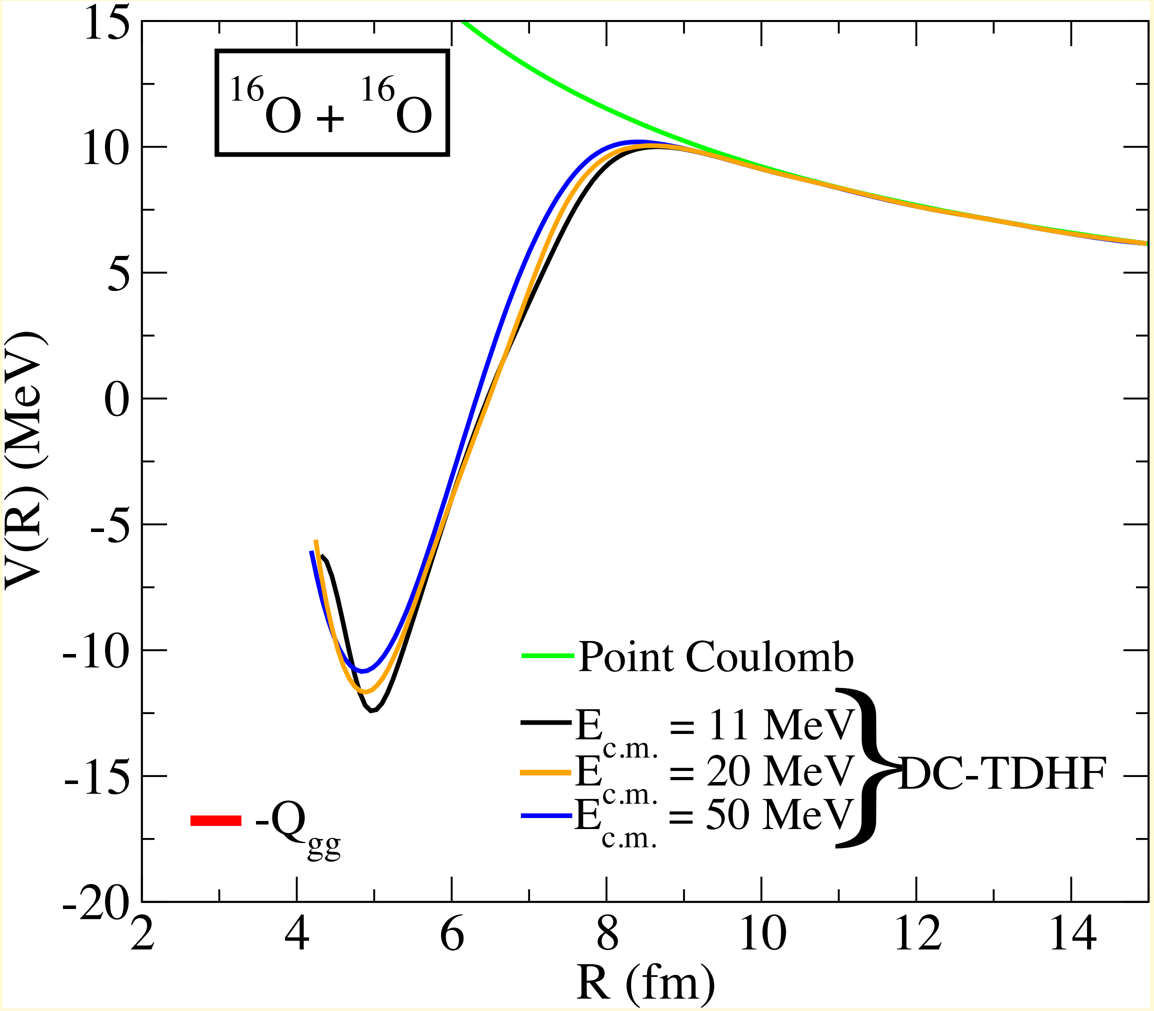
$^{16,24}O + ^{16,24,28}O$ and $^{16,18,19,20,24}O + ^{12}C$

Sub-barrier fusion: relevant for neutron star crust !

- Umar, Oberacker & Horowitz, PRC 85, 055801 (2012)
- Umar, Oberacker, Maruhn & Keser: Proc. Sanibel conf. (2012)
- deSouza, Hudan, Oberacker & Umar, PRC 88, 014602 (2013)

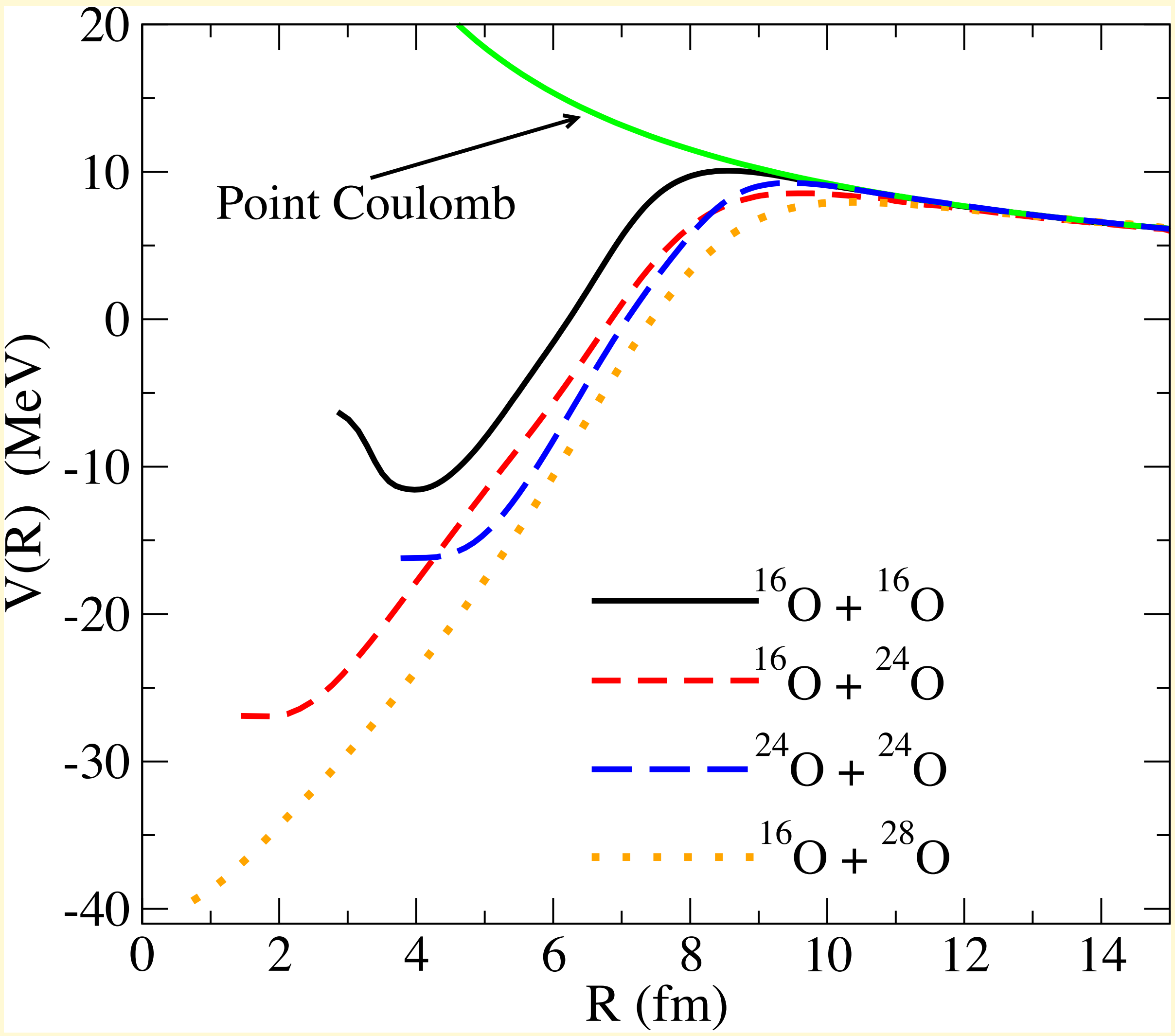
V(R) for light systems: weak dependence on E_{cm}

Ref: Umar, Oberacker, Maruhn & Reinhard, PRC 80, 041601(R) (2009)



heavy-ion potentials for oxygen isotopes

Ref: Umar, Oberacker & Horowitz, PRC 85, 055801 (2012)

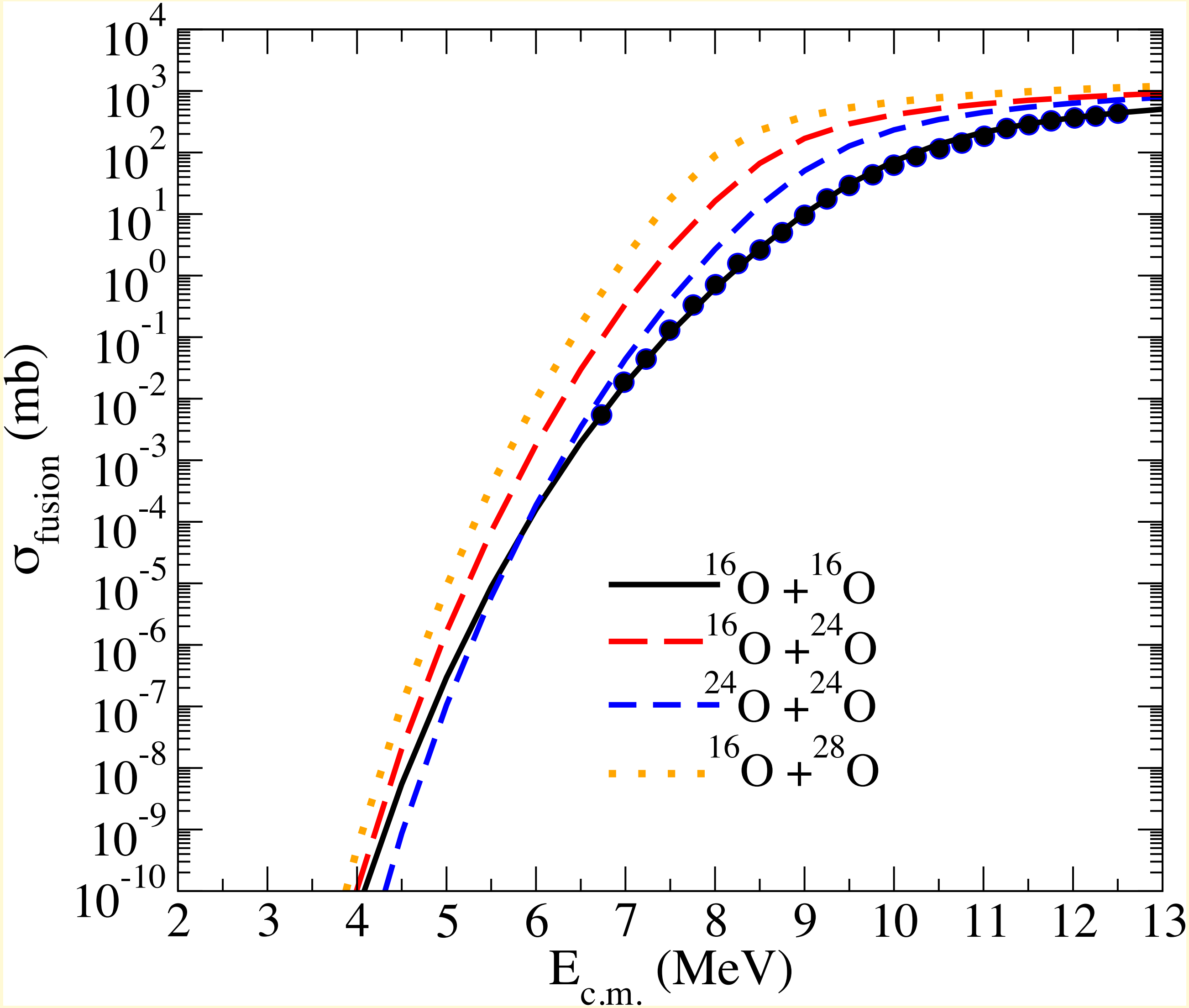


barrier heights (MeV)

10.00
9.24
8.54
7.95

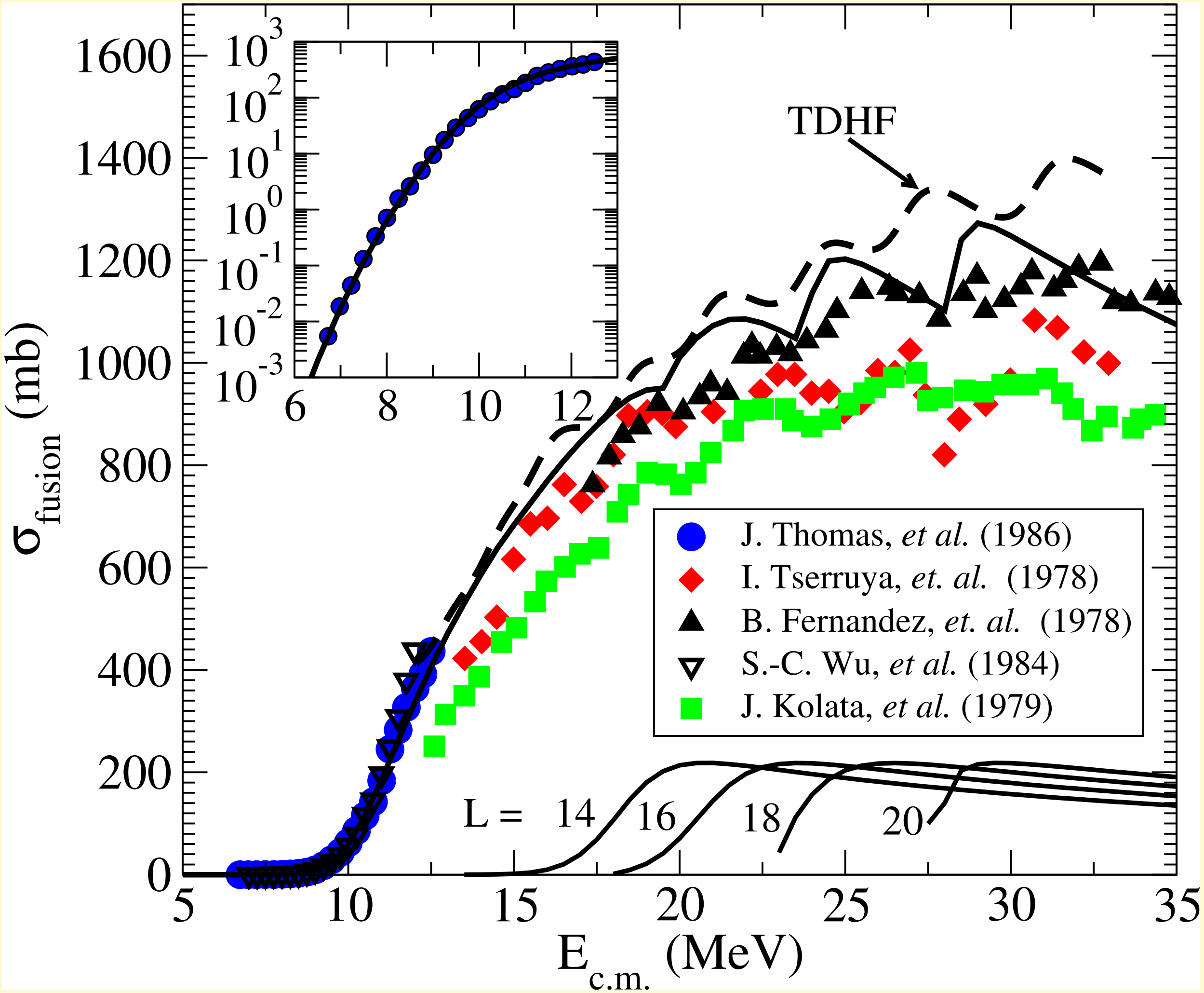
total fusion cross sections for oxygen isotopes

Ref: Umar, Oberacker & Horowitz, PRC 85, 055801 (2012)



$^{16}O+^{16}O$ fusion at higher energies (up to $E=3.5\ E_{coul}$)

Ref: Simenel, Keser, Umar & Oberacker, PRC 88, 024617 (2013)



We need new experiments !

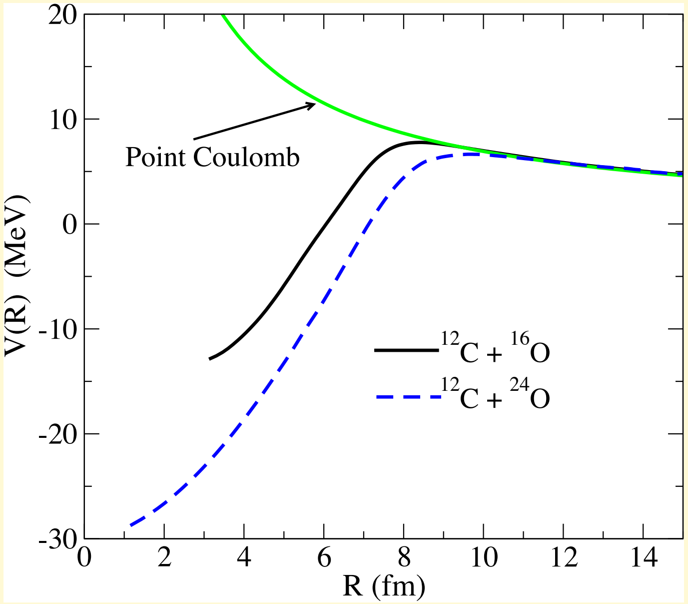
excellent test case for current and future microscopic theories:

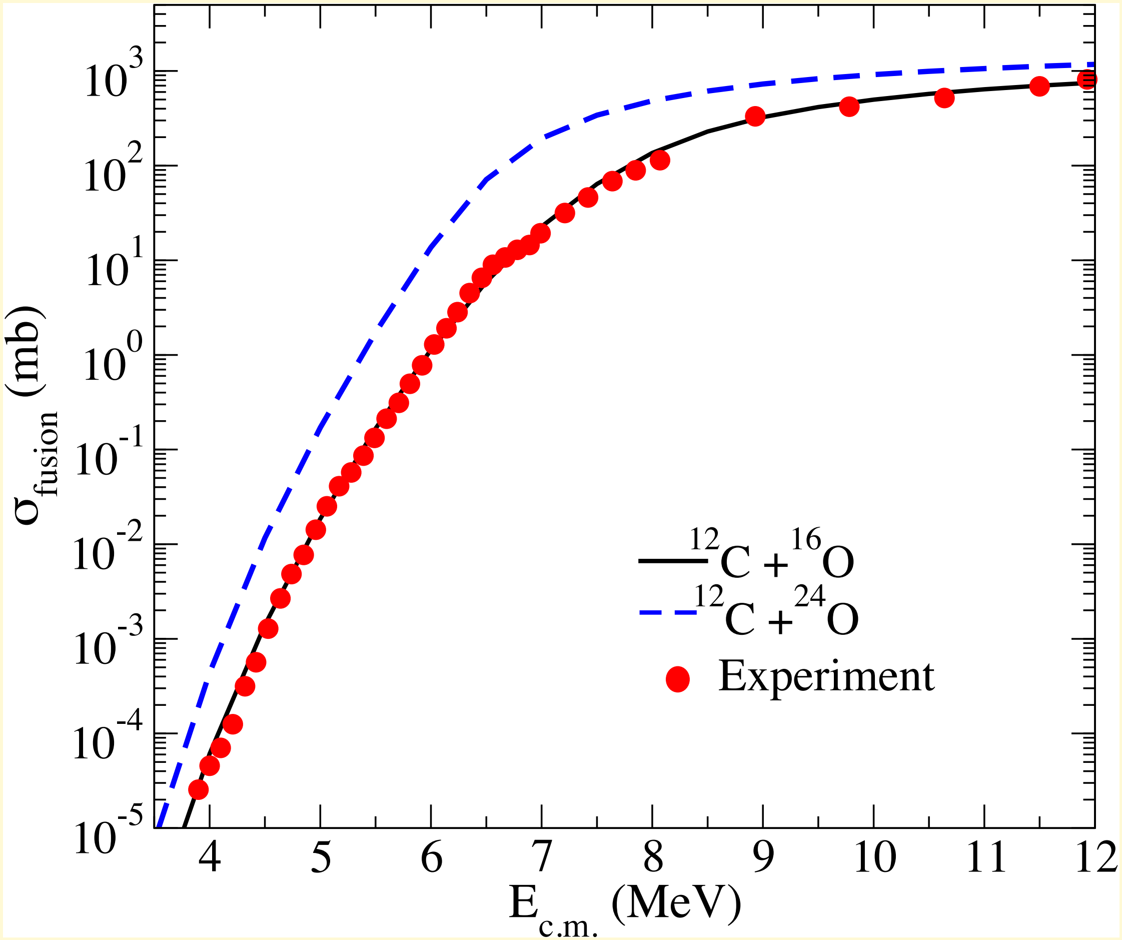
- ^{16}O in most Skyrme force fits
- doubly magic (no pairing issues)
- light system (small CPU time)

Similar results and conclusions: Esbensen, PRC 77, 054608 (2008)

$^{12}C + ^{16,24}O$ fusion

Ref: Umar, Oberacker & Horowitz, PRC 85, 055801 (2012)



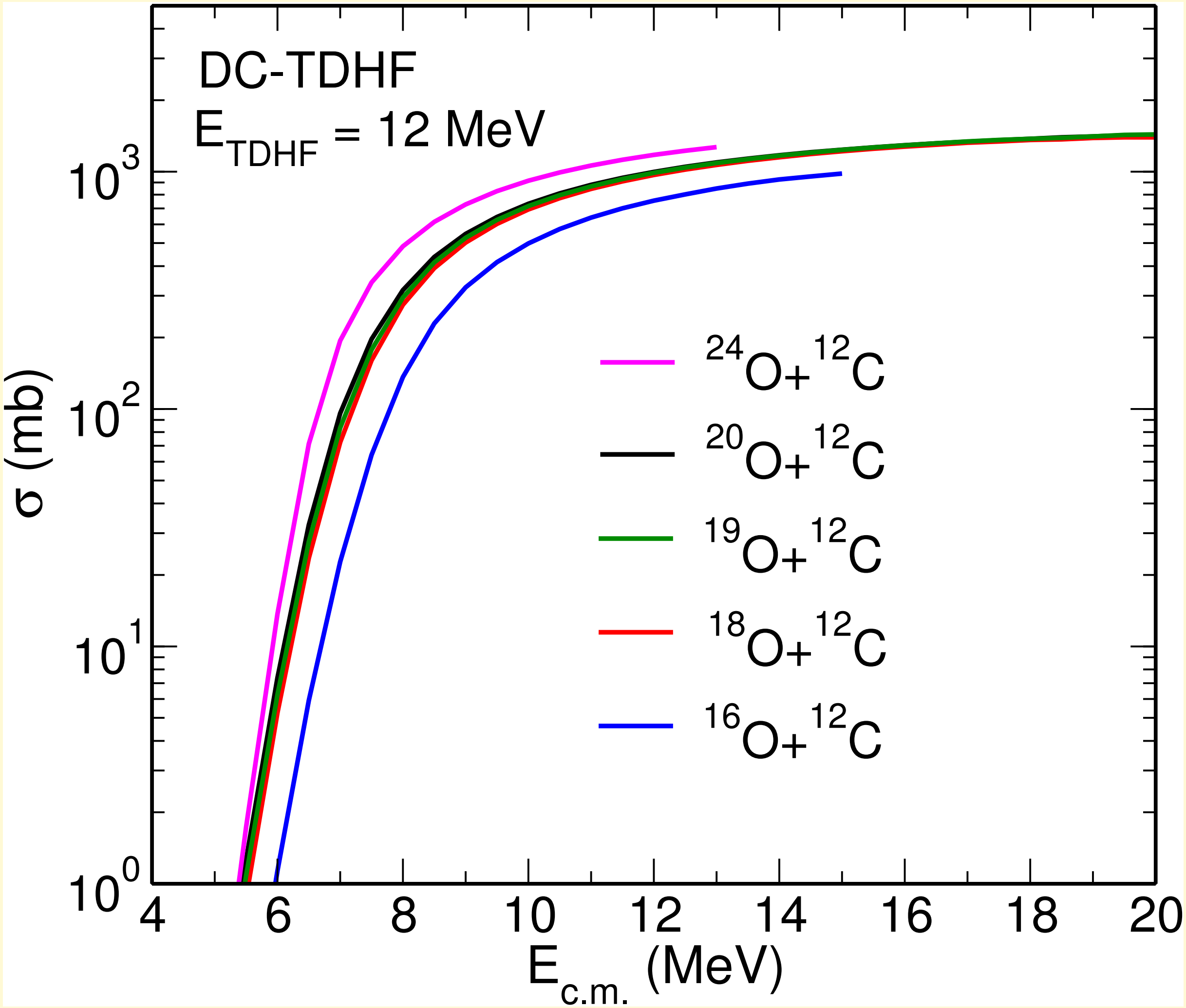


barrier heights (MeV)

7.77

6.64

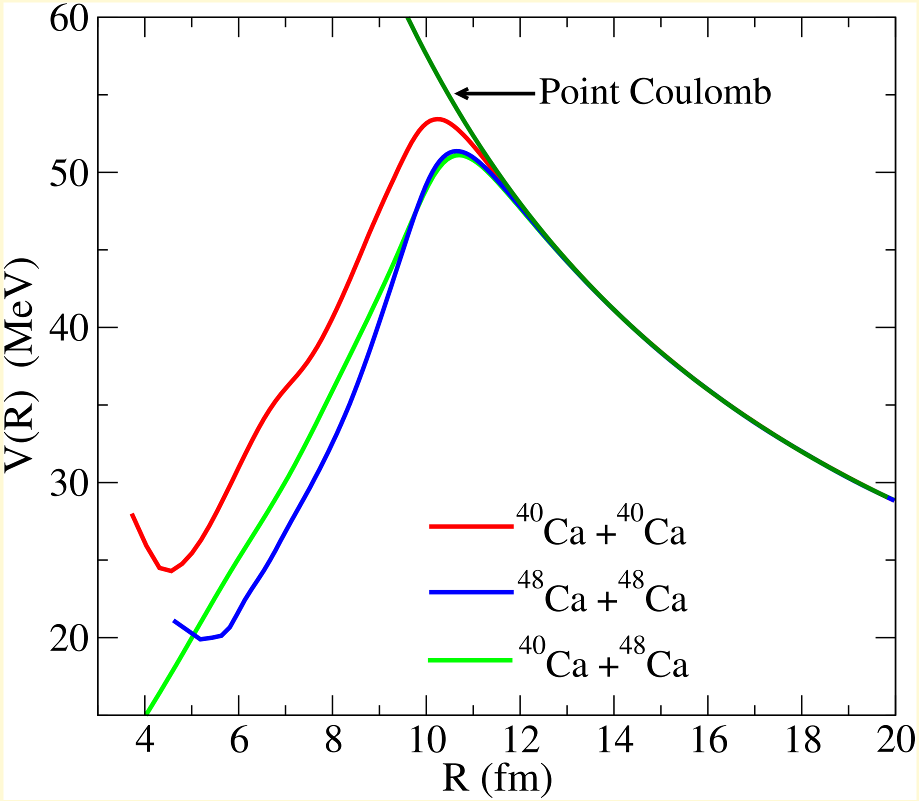
DC-TDHF predictions for $^{18,19,20}O+^{12}C$

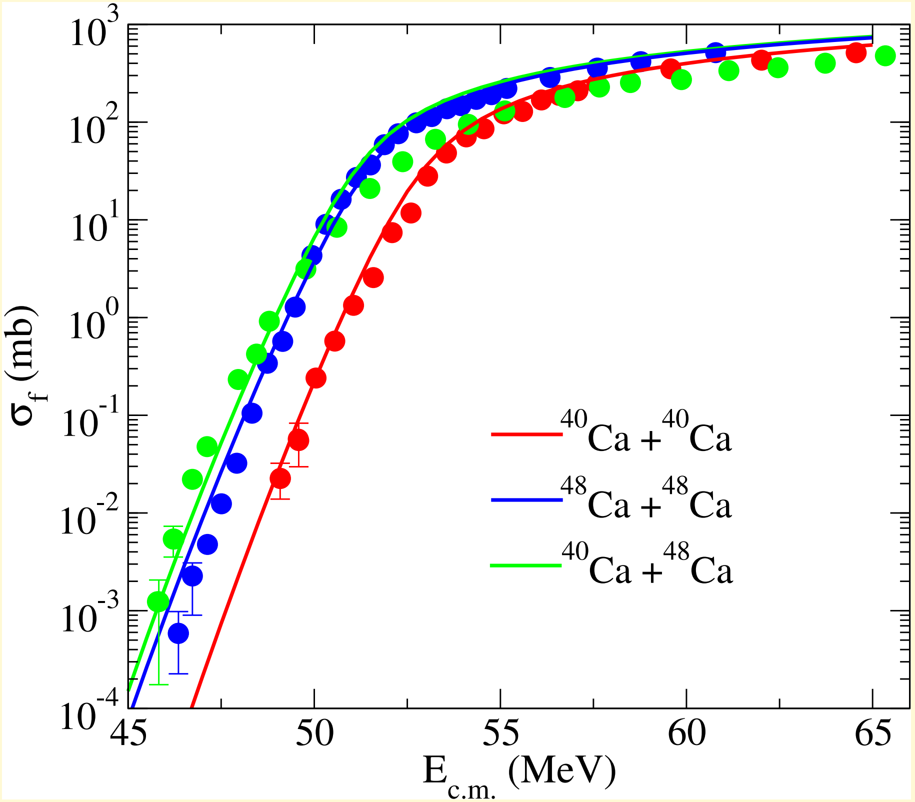


Fusion experiments are scheduled for
Fall 2013 / Spring 2014
at Florida State Univ.
(deSouza et al.)

Sub-barrier fusion of $^{40,48}Ca + ^{40,48}Ca$

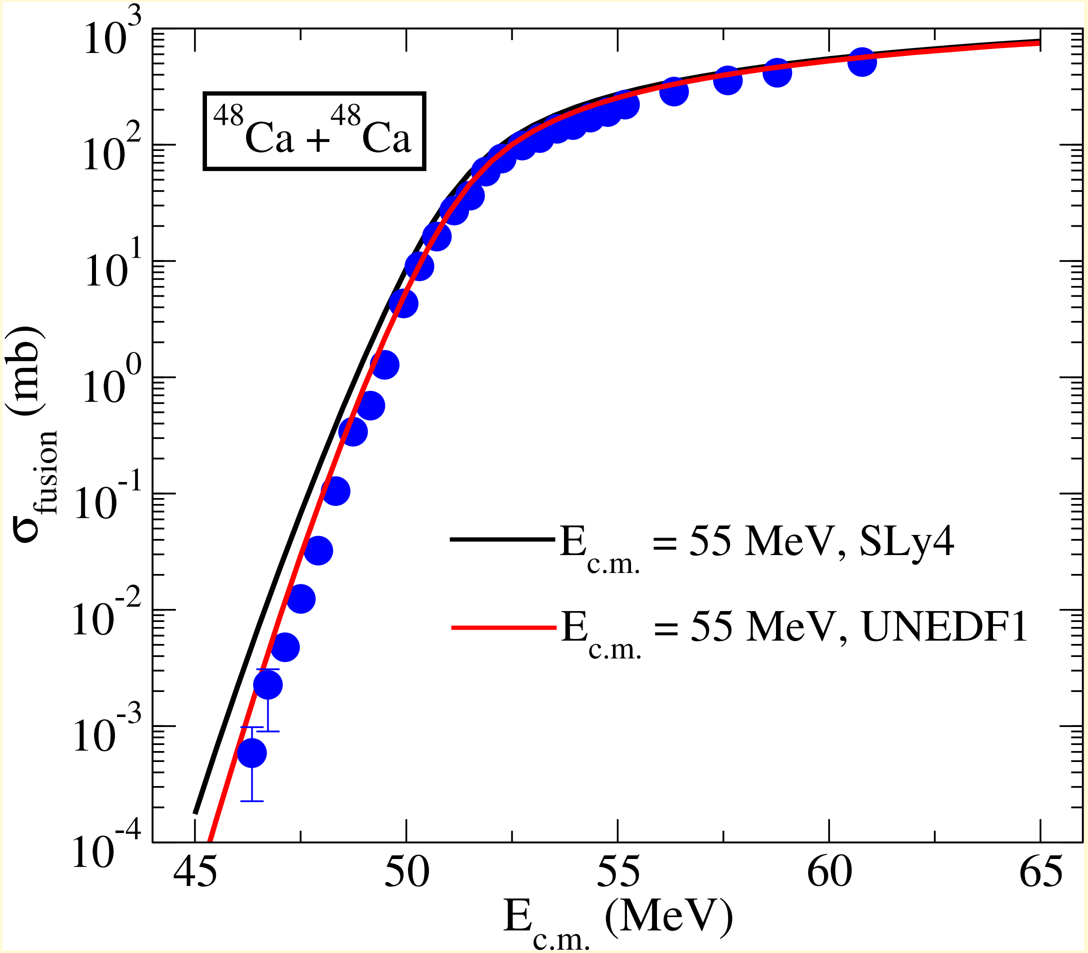
Keser, Umar, and Oberacker, PRC 85, 044606 (2012)





Sub-barrier fusion of $^{48}Ca + {}^{48}Ca$

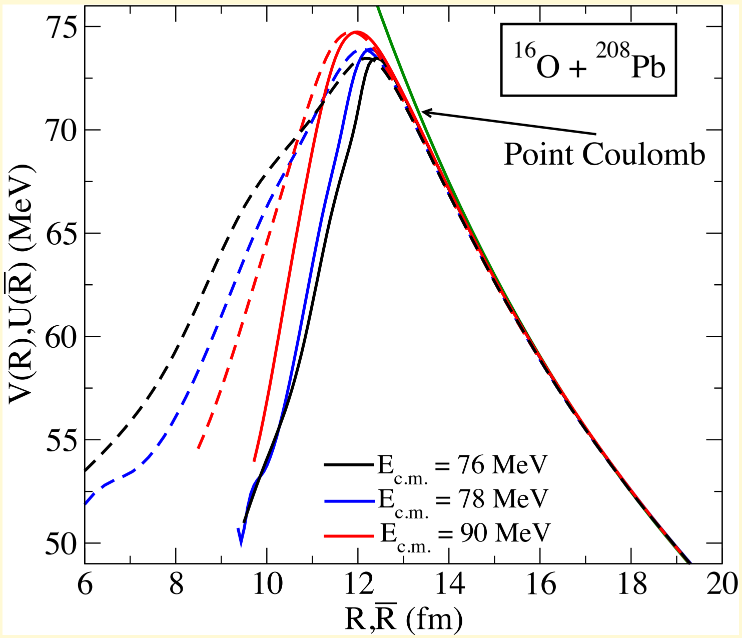
Keser, Umar, and Oberacker, PRC 85, 044606 (2012)

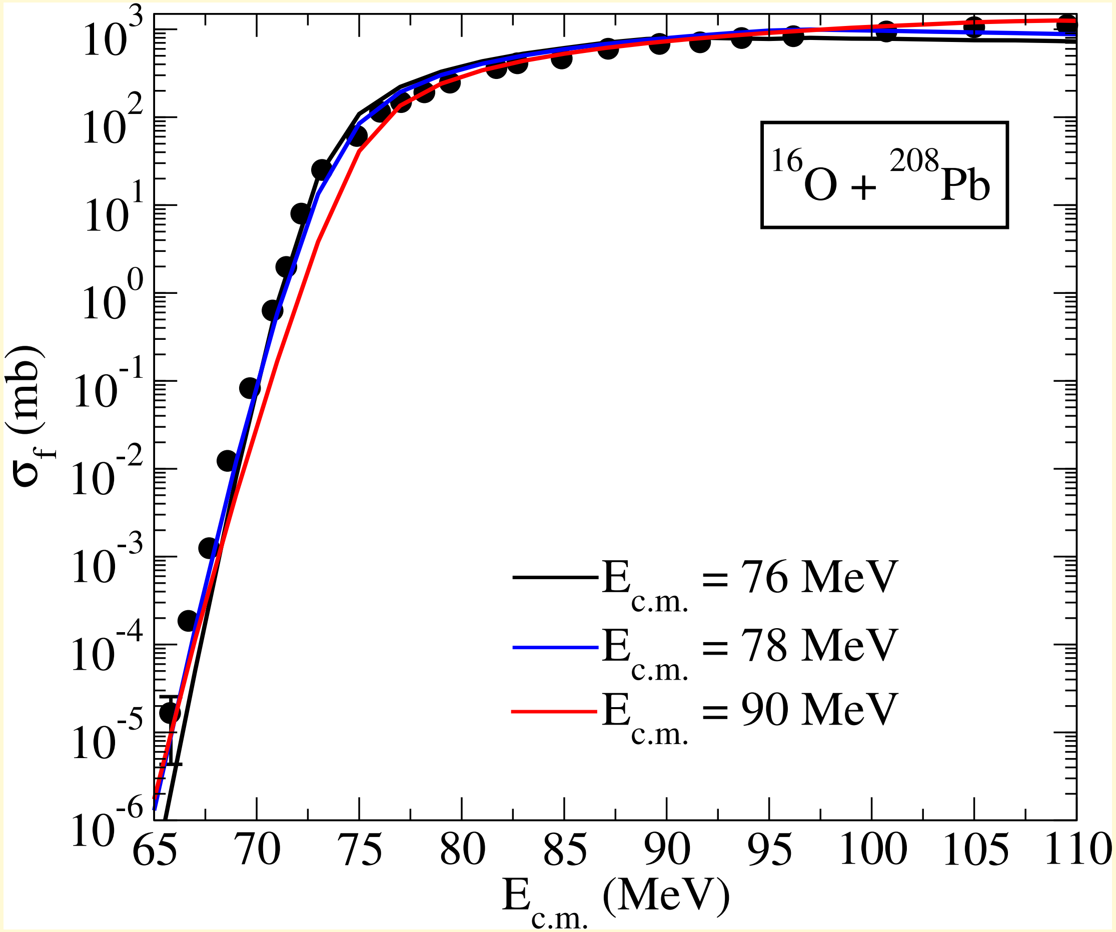


used two Skyrme forces:
SLy4 and UNEDF1

$^{16}O + ^{208}Pb$ fusion

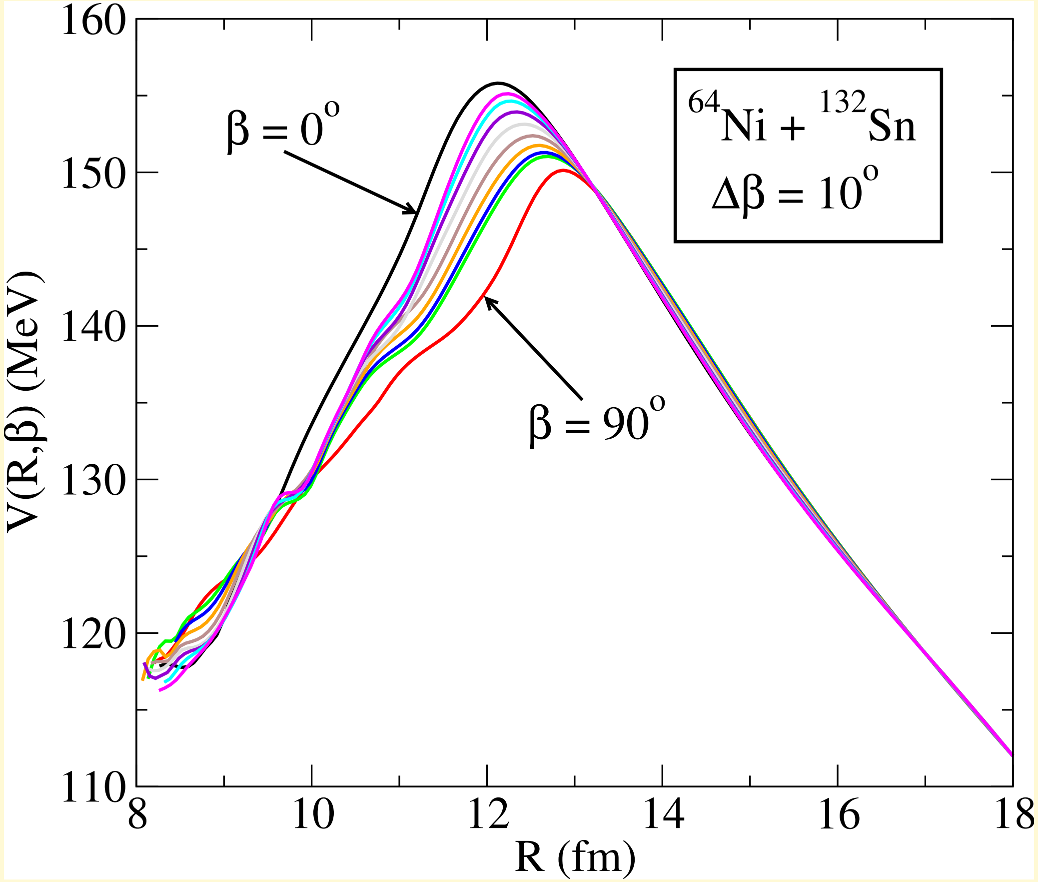
Umar and Oberacker, Eur. Phys. J. A 39, 243 (2009)

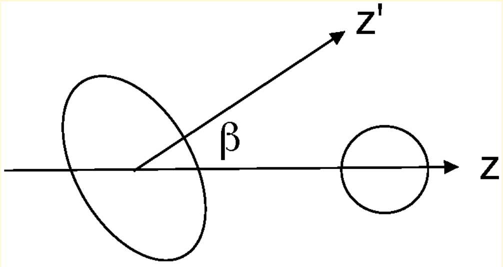




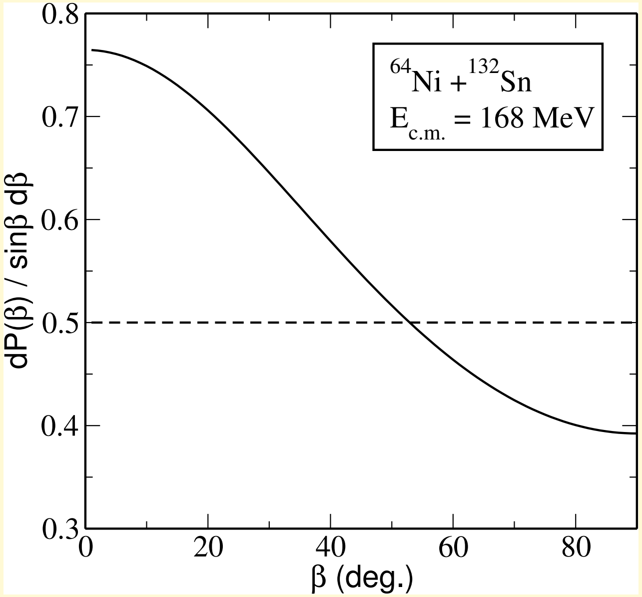
Spherical + deformed (oblate) nucleus: $^{132}Sn + ^{64}Ni$

Umar & Oberacker, PRC 76, 014614 (2007)

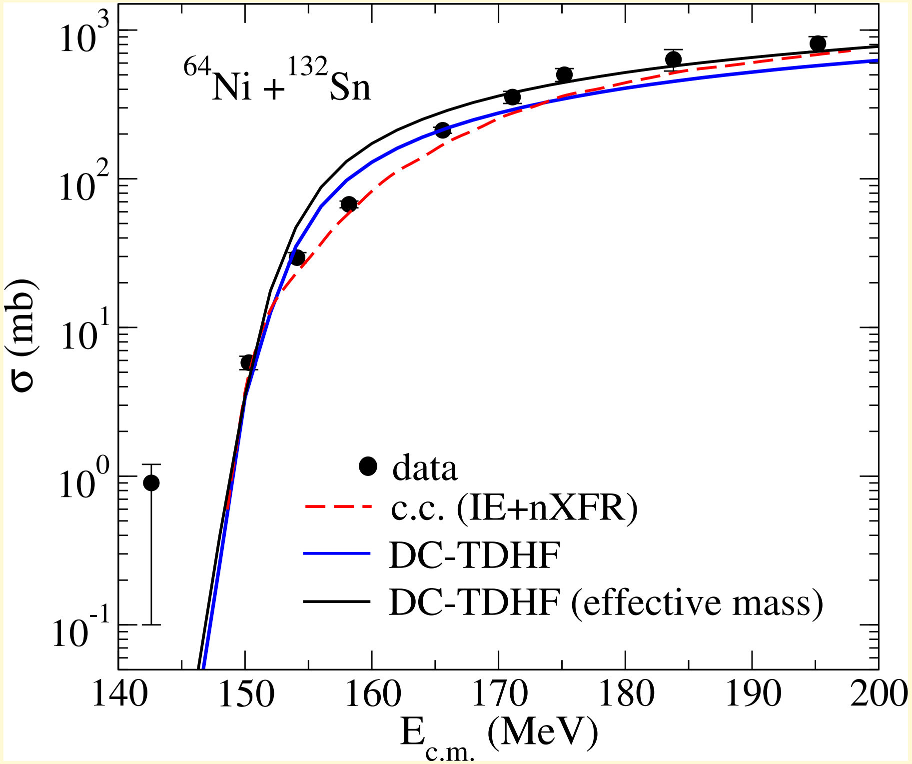


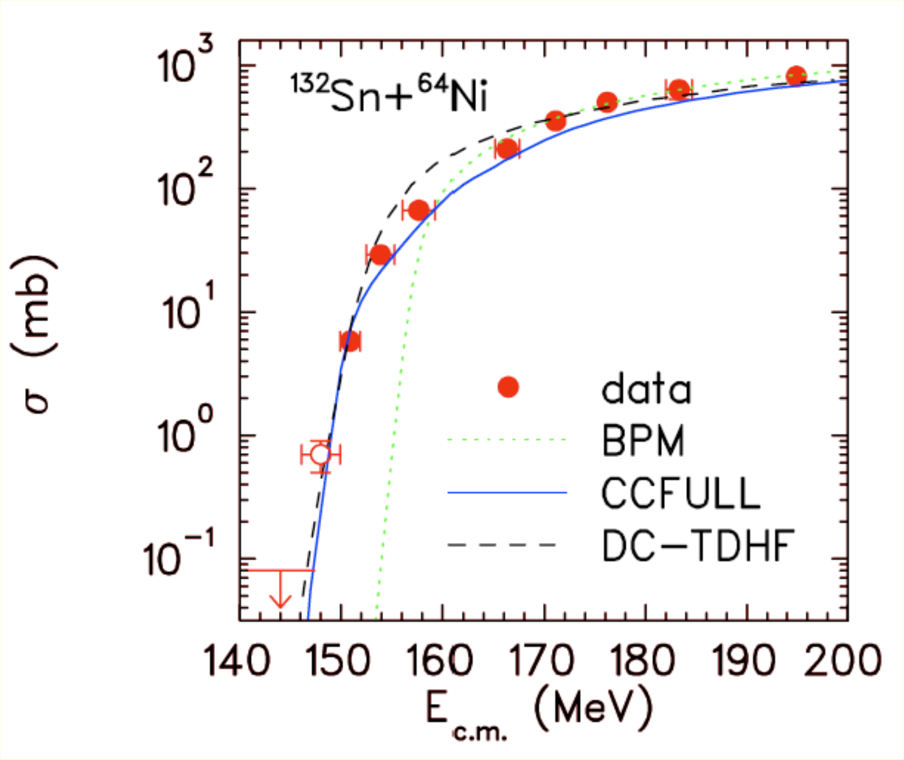


Heavy-ion potential depends on initial orientation angle β of deformed nucleus



^{64}Ni + ^{132}Sn sub-barrier fusion: first reaction studied with DC-TDHF



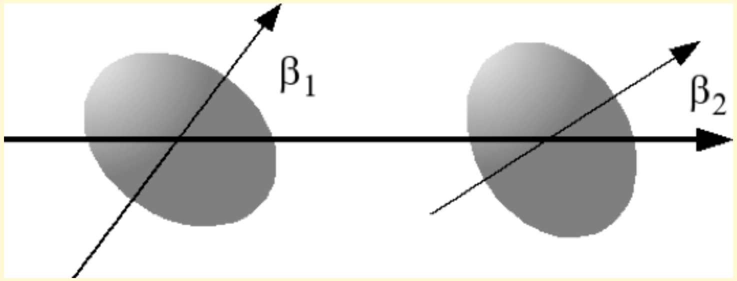


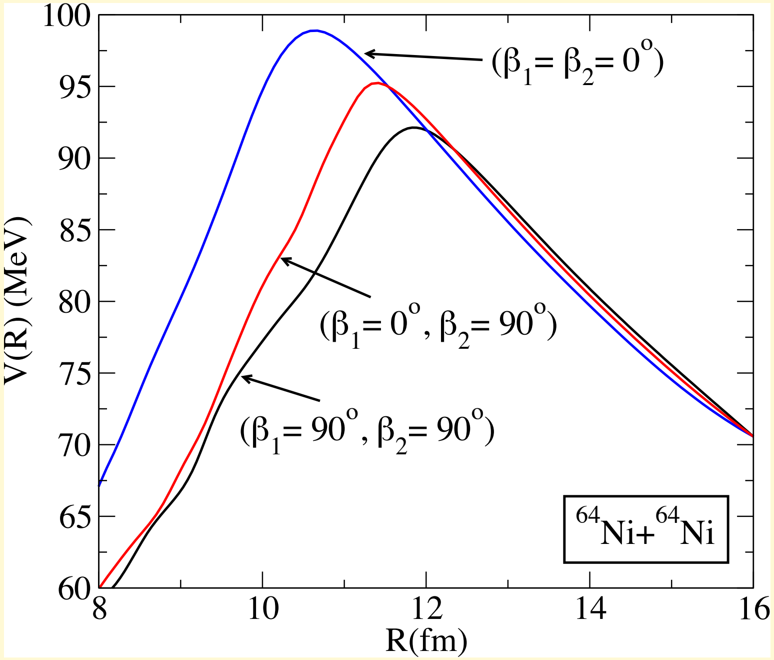
DC-TDHF theory
Umar and Oberacker,
PRC 76, 014614 (2007)

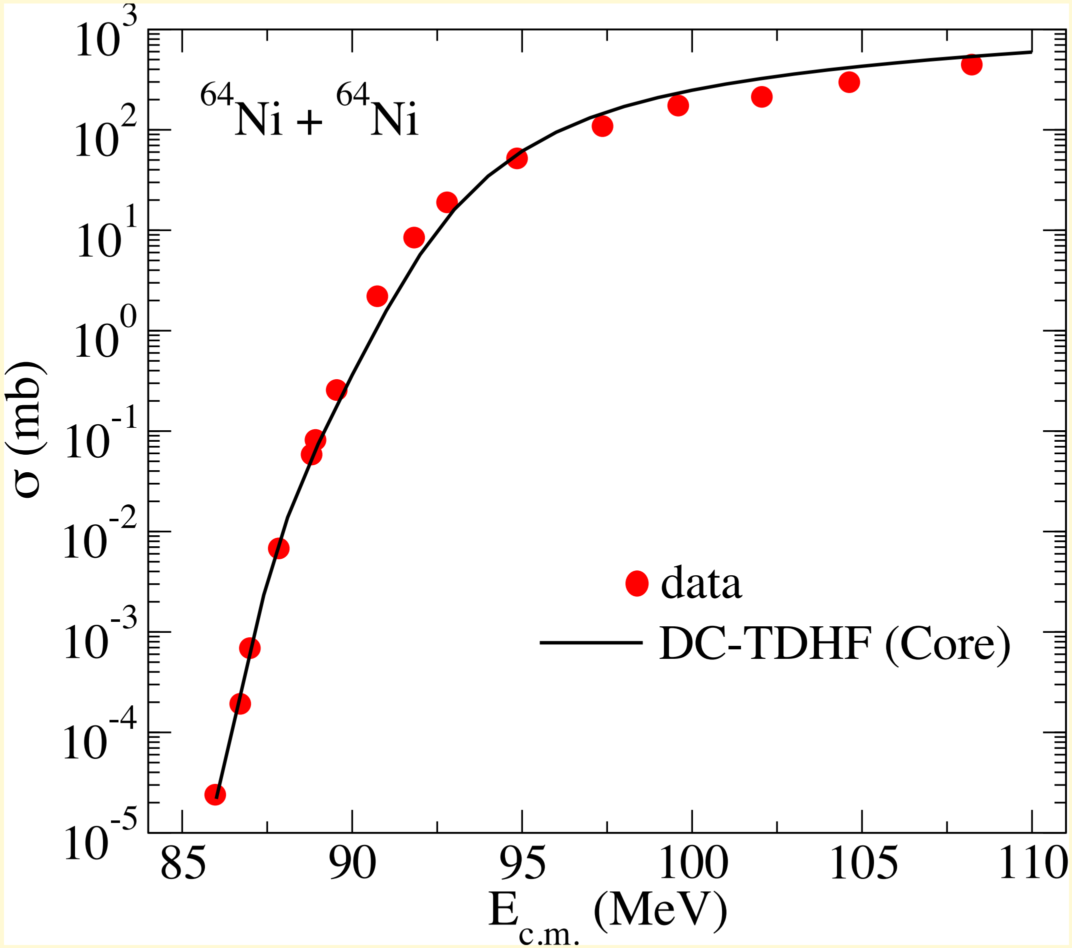
Exp. Data (HRIBF, ORNL)
J.F. Liang et al.,
PRL 91, 152701 (2003)
PRC 75, 054607 (2007)
PRC 78, 047601 (2008)

Fusion hindrance in ^{64}Ni + ^{64}Ni

Umar and Oberacker, Phys. Rev. C 77, 064605 (2008)



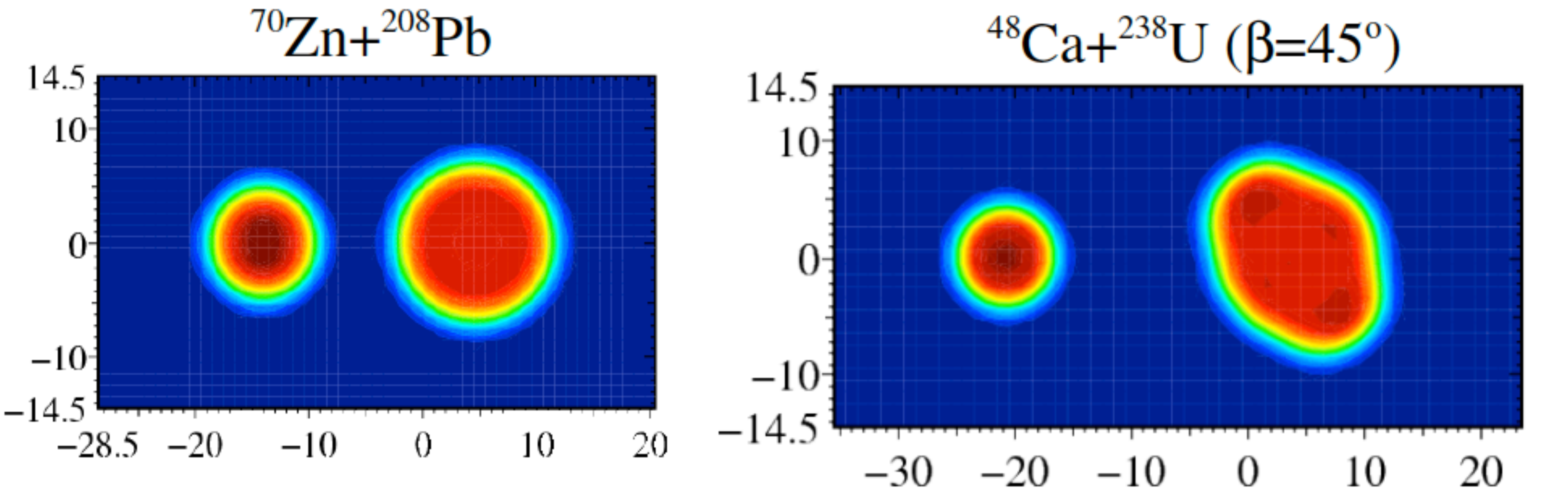




Heavy-ion fusion leading to superheavy element Z=112

spherical + spherical:
“cold fusion” (E* small)

spherical + deformed:
“hot fusion” (E* large)



Factors Influencing Superheavy Formations

- Excitation energy
  high excitation at the capture configuration → quasi-fission
  high excitation of compound nucleus → fusion-fission
- Nuclear deformation and alignment
- Shell effects
- Mass asymmetry in the entrance channel
- Impact parameter dependence
- ......

$$\sigma_{ER} = \sigma_{capture} \cdot P_{CN} \cdot P_{survival}$$

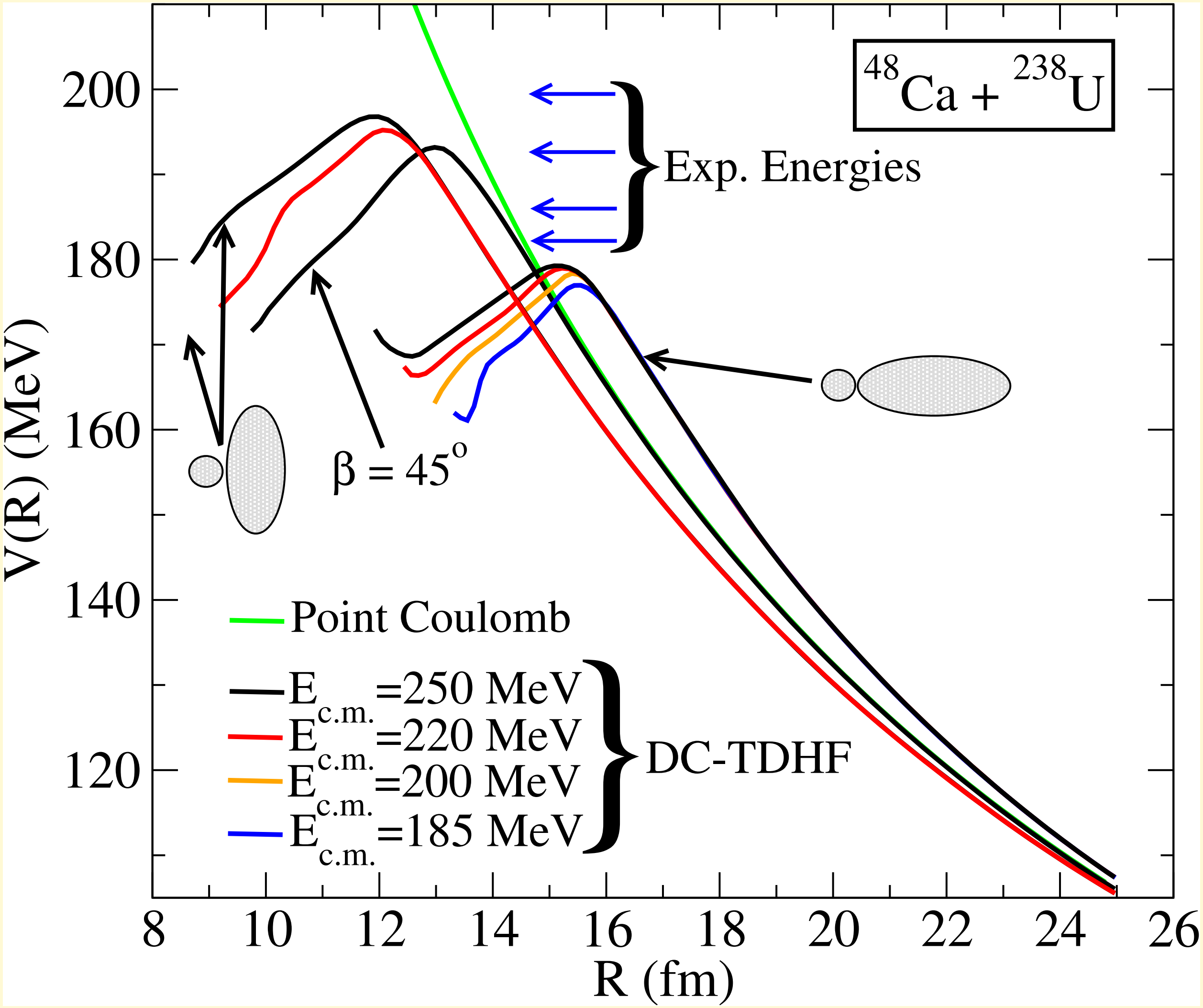
Capture in ion-ion potential pocket

Form compound system

Survive FF process

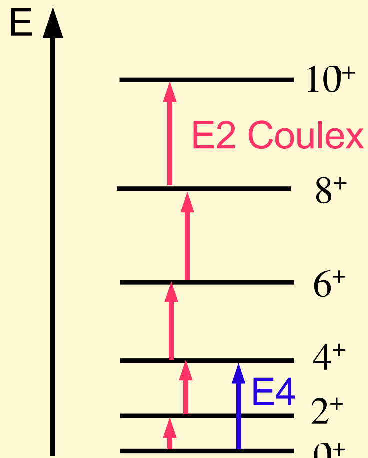
$^{48}Ca + ^{238}U$ internuclear potential

Umar, Oberacker, Maruhn & Reinhard, PRC 81, 064607 (2010)

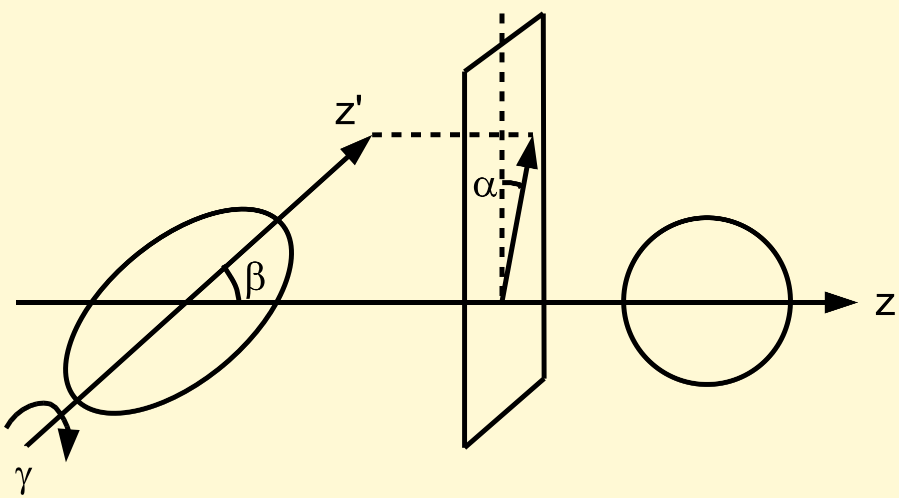


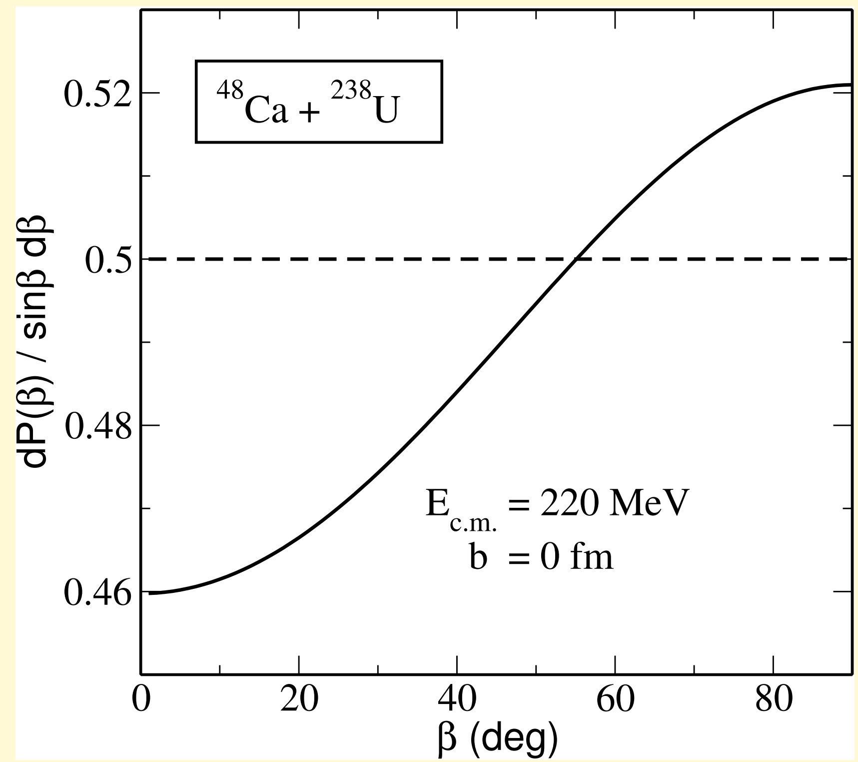
Dynamic alignment (due to Coulex) of ^{238}U in hot fusion

Umar, Oberacker, Maruhn & Reinhard, PRC 81, 064607 (2010)



K=0 rotational band



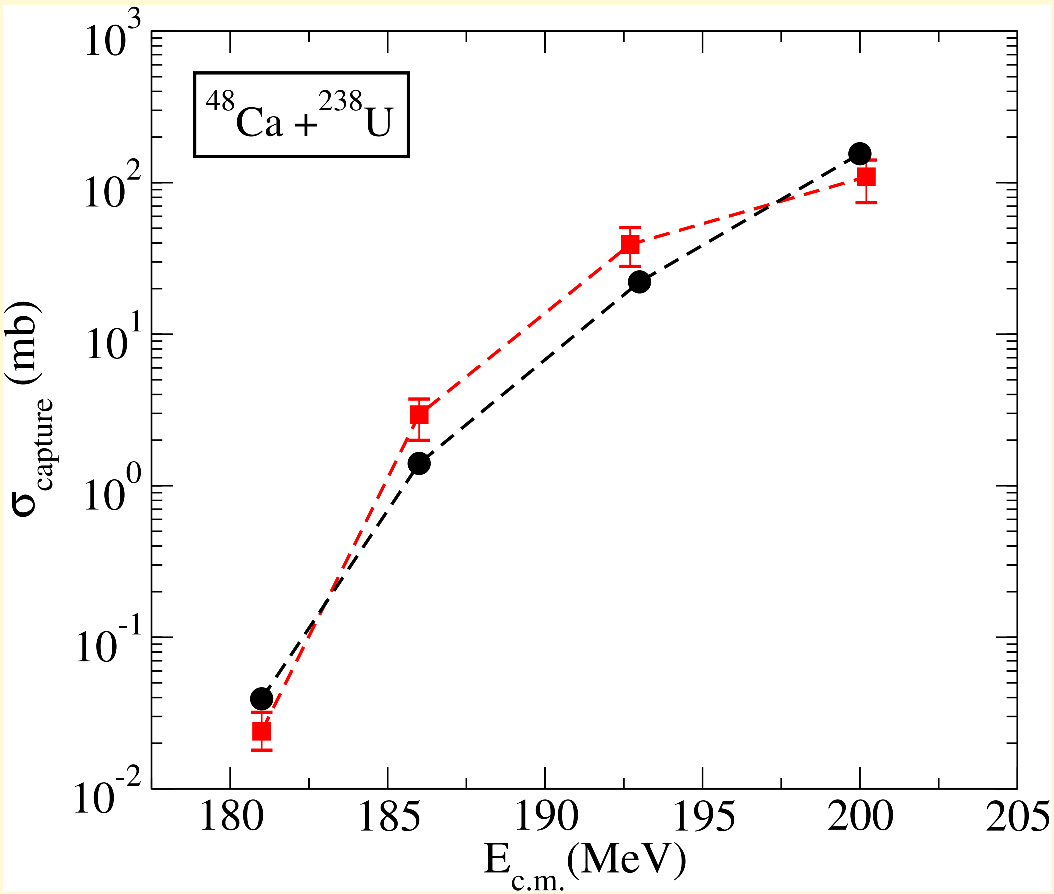


$^{48}Ca + {}^{238}U$ capture cross section

Umar, Oberacker, Maruhn & Reinhard, PRC 81, 064607 (2010)

$$\sigma_{capt}(E_{cm}) = \int_0^{\pi} \sin\beta d\beta \frac{dP(\beta)}{\sin\beta d\beta} \sigma_{capt}(E_{cm}, \beta)$$

dynamic alignment

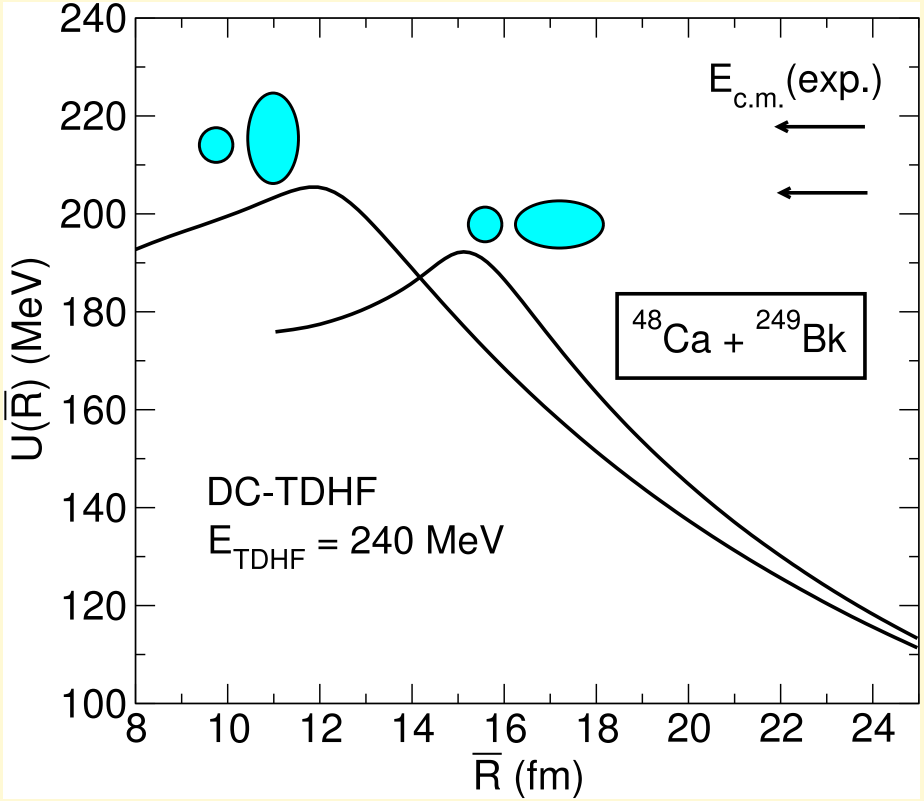


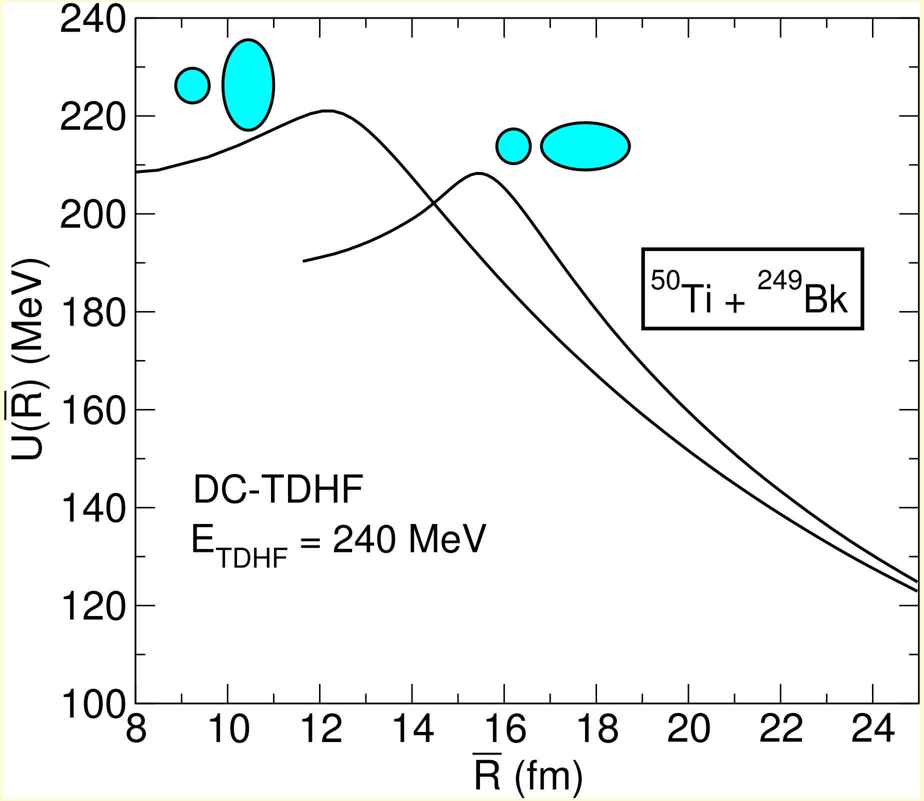
- σ(β) decreases rapidly for β>10°
- sin(β) multiplies small angles
- dP(β) is in the range 0.46 - 0.52

● DC-TDHF

■ Experiment: Oganessian *et al.*, J. Phys. G 34 R165 (2007)

Comparison: internuclear potentials for $^{48}Ca, ^{50}Ti + ^{249}Bk$





exp: DGFRS Dubna
σ (Z=117) = 1.1-2.4 pb
50 times larger !

exp: TASCA GSI
σ (Z=119) < 50 fb

Summary

- DC-TDHF: time-dependent density functional theory for fusion below and above the barrier

- only input: Skyrme N-N interaction, no adjustable parameters

- DC-TDHF output:
  internuclear potential V(R), mass M(R), fusion cross section σ(E), excitation energy E*(R), average multi-nucleon transfer, pre-equilibrium GDR excitation and dipole radiation

- Quantitative sub-barrier fusion calculations are now possible, detailed comparison with experimental data (about 25 fusion reactions studied with DC-TDHF between 2006 -2013)

- Grand Challenge: include pairing into DC-TDHF
  develop TDHFB code on 3D lattice for nuclear reactions

Current research projects

- Neutron star crust: fusion reactions (C+O, O+O) in the presence of a neutron gas with variable density
collaboration with Charles Horowitz and P.-G. Reinhard

- Fusion of light systems ($^{18,19,20}O+^{12}C$): DC-TDHF calculations finished, fusion experiments in Fall 2013 / Spring 2014 at Florida State, collaboration with experimentalists at Indiana University (Romualdo deSouza et al.)

- Studies in connection with superheavy element formation:
a) DC-TDHF capture cross sections for ^{48}Ca,^{50}Ti + ^{249}Bk
b) Quasifission in ^{50}Ti + ^{208}Pb, ^{48}Ca + ^{248}Cm, …
unrestricted TDHF, possible collaboration with Cedric Simenel
experimental guidance by Zach Kohley and Walt Loveland