Connecting fundamental models with nuclear reaction evaluations

G. P. A. Nobre

National Nuclear Data Center

Brookhaven National Laboratory

Workshop at Institute for Nuclear Theory, March 13-17, 2017

Nuclear Reactions: A Symbiosis between Experiment, Theory and Aplications

BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

Summary

- What is a reaction evaluation?
- Importance of predictive theory in reaction evaluations
  - Extrapolation
  - Compensation of errors
- Soft-rotor optical potential applied to Iron evaluations
- Coupled-channels on interpolated Optical Potentials
  - Adiabatic principle: Separation of degrees of freedom
  - Rare-earth angular distributions
- Reaction observables from microscopic transition densities/potentials for nucleon-nucleus reactions
  - Reaction cross sections
  - Total cross sections
  - Angular distributions

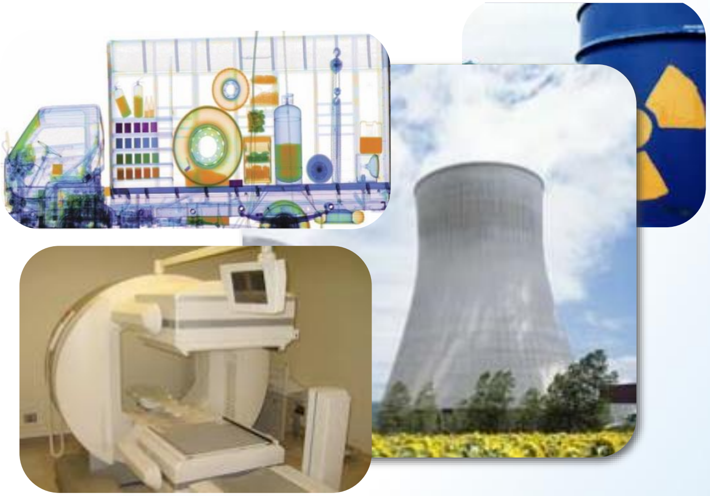
Summary

- What is a reaction evaluation?
- Importance of predictive theory in reaction evaluations
  - Extrapolation
  - Compensation of errors
- 1 Soft-rotor optical potential applied to Iron evaluations
- 2 Coupled-channels on interpolated Optical Potentials
  - Adiabatic principle: Separation of degrees of freedom
  - Rare-earth angular distributions
- 3 Reaction observables from microscopic transition densities/potentials for nucleon-nucleus reactions
  - Reaction cross sections
  - Total cross sections
  - Angular distributions

The Nuclear Data Community is the link between basic science and applications

Nuclear Science Community

- Experiments
- Theory



Nuclear Data Community

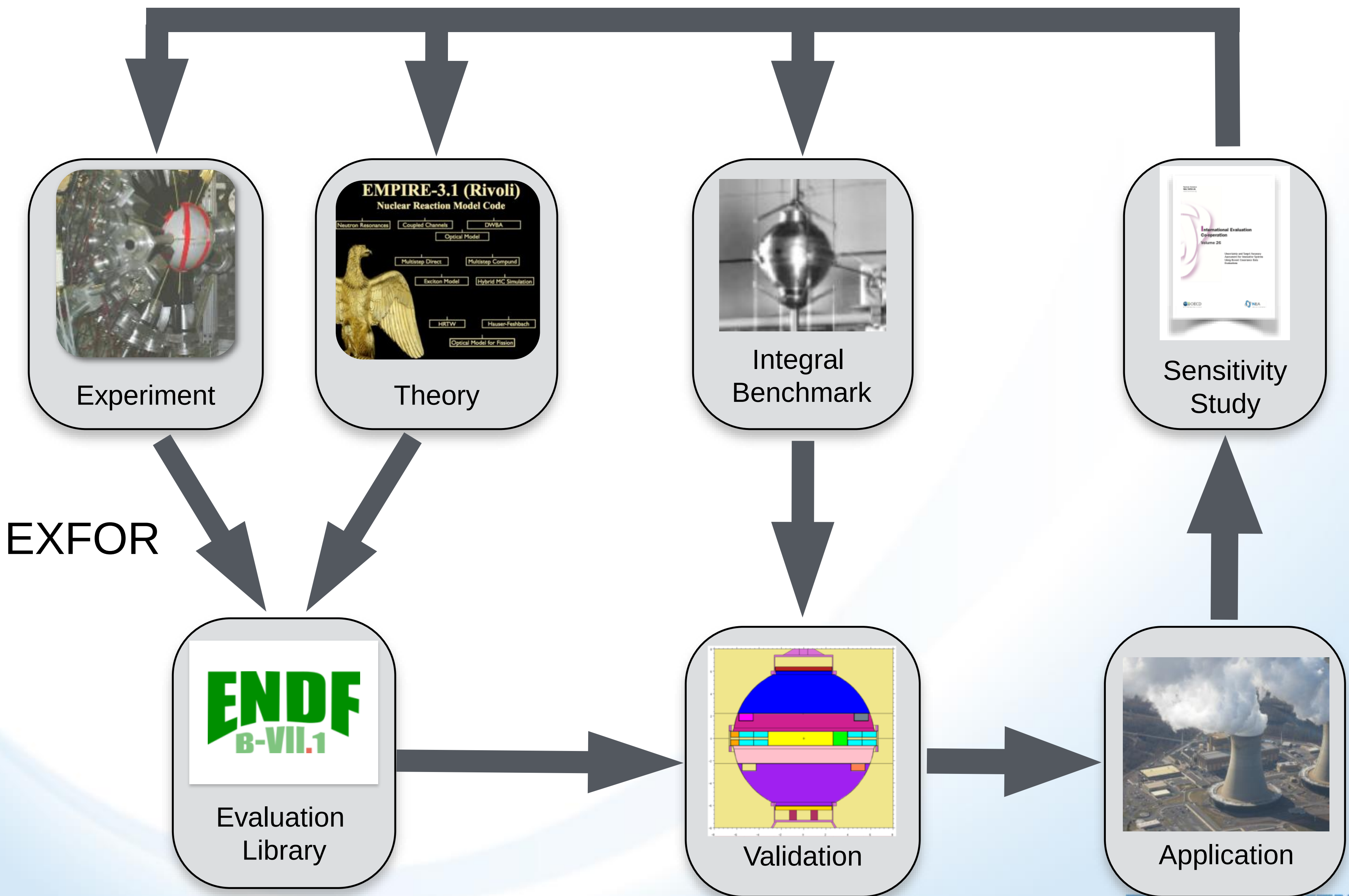
- Compilation
- Evaluation
- Dissemination
- Archival

Application Community needs data:

- Complete
- Organized
- Traceable
- Readable

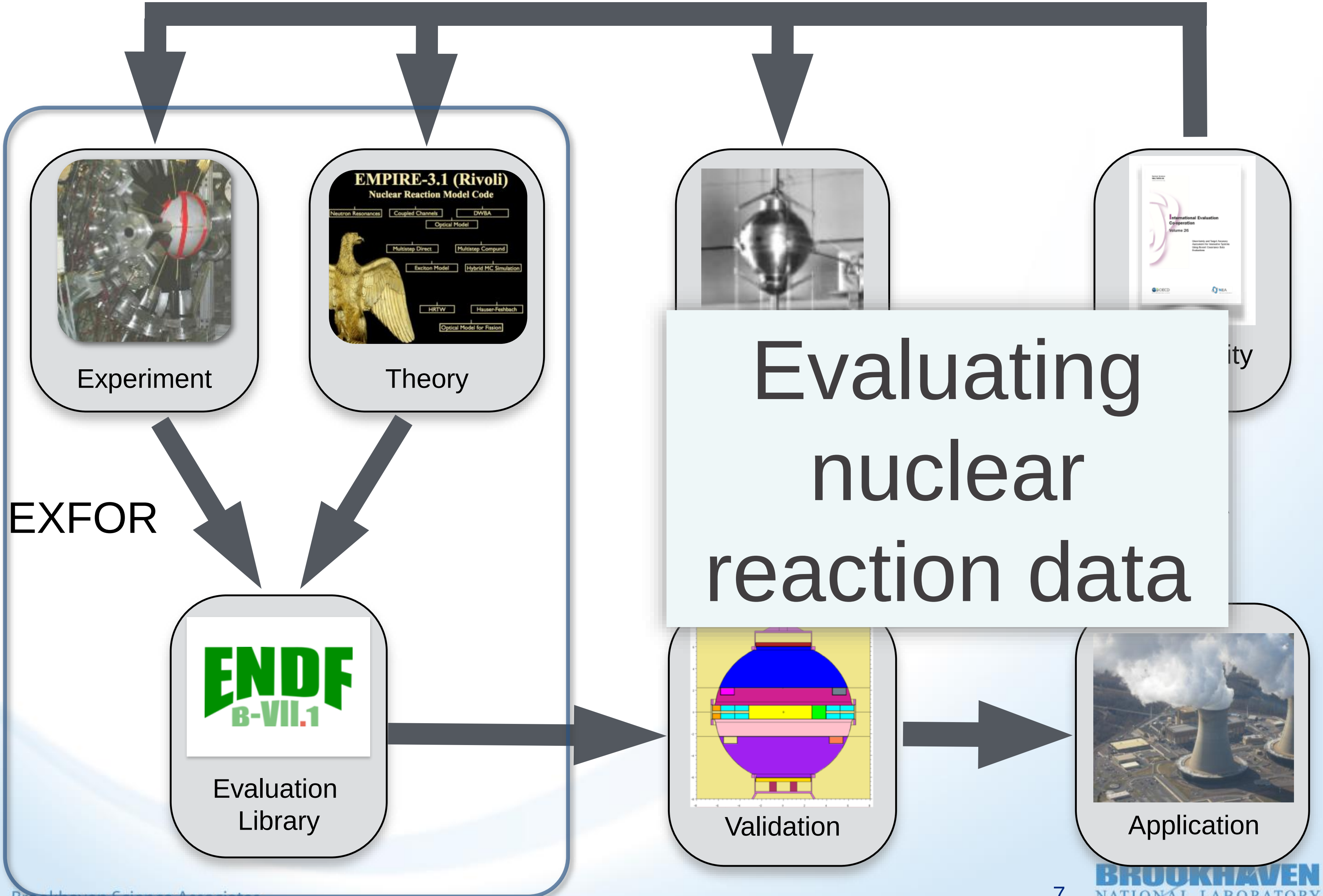
Reaction evaluations

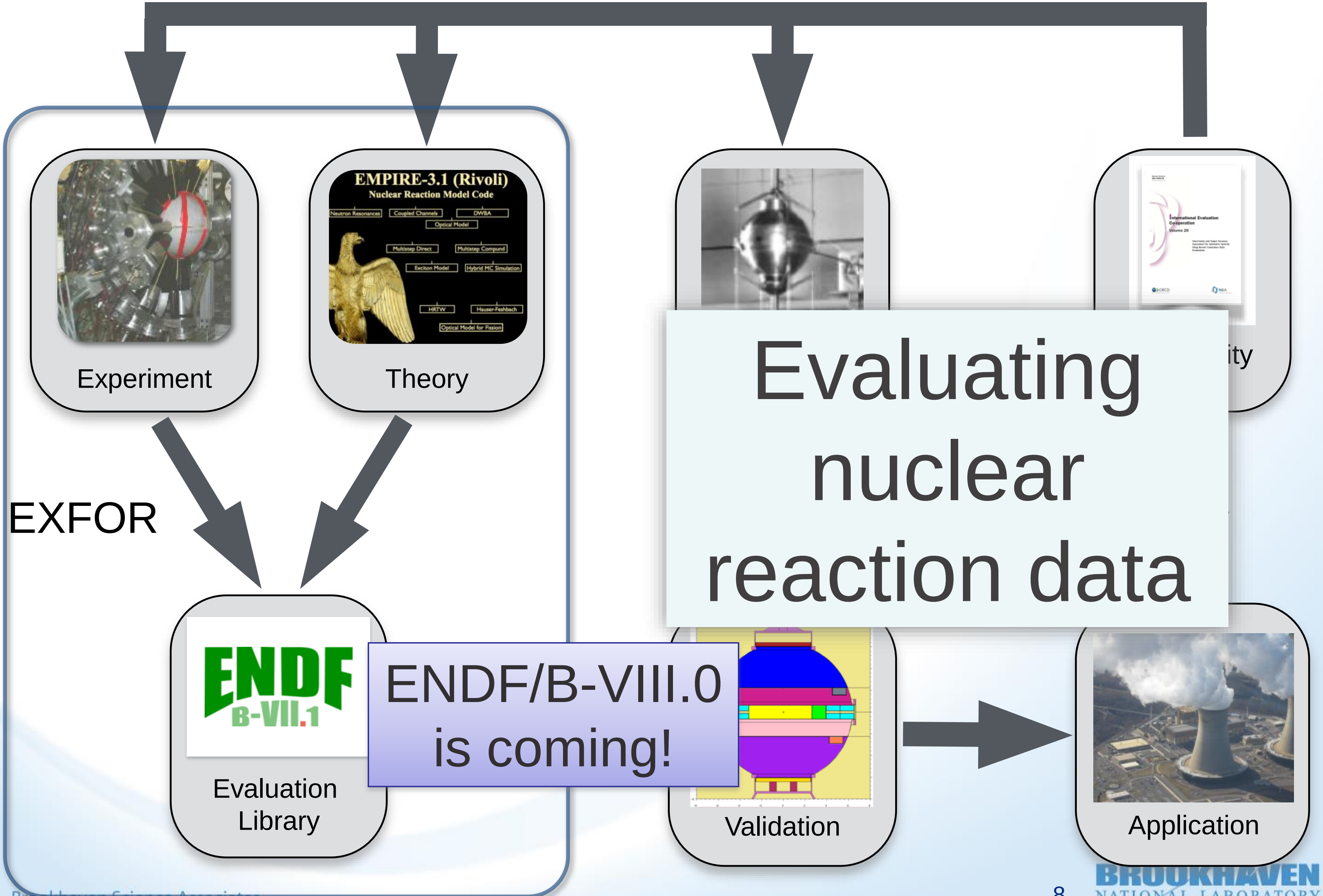
- Goal: Provide best cross sections (integrated/differential)
- Used in applications: Nuclear power, astrophysics, medical isotope production, national security...
- Sub-libraries: neutron, proton, decay, ...
- Analysis of experimental data
  - Conflicting sets
  - Always be incomplete
- Modeling fills gaps
- Validation (integral testing)
  - Critical assemblies
  - Normally only one quantity is measured
  - Compensation of errors
  - Examples: minor Iron isotopes, Cromium issue in steel, etc.



EMPIRE-3.1 (Rivoli)
Nuclear Reaction Model Code
Neutron Resonances
Coupled Channels
DWBA
Optical Model
Multistep Direct
Multistep Compound
Exciton Model
Hybrid MC Simulation
HRTW
Hauser-Feshbach
Optical Model for Fission
Experiment
Theory
Integral
Benchmark
Sensitivity
Study
EXFOR
ENDF
B-VII.1
Evaluation
Library
Validation
Application

Evaluating nuclear reaction data




EMPIRE-3.1 (Rivoli)
Nuclear Reaction Model Code
Experiment
Theory
EXFOR
ENDF
B-VII.1
Evaluation
Library
ENDF/B-VIII.0
is coming!
Evaluating
nuclear
reaction data
Validation
Application

Soft-Rotator Model (SRM)

1

- SRM used to obtain a dispersive OP: Fe evaluation
- Collective models are normally assumed either pure rotational or vibrational
- However, "centrifugal" forces in some rotating nuclei lead to displacement of nuclear matter within the nucleus
- Vibration within deformed matter: "Softness" parameter
- Applied to light, medium, and heavy nuclei, which are not pure vibrational nor pure rotors

$$R_i(\theta',\varphi') = R_{0i}\left\{1 + \sum_{\lambda=2,4,6,8} \beta_{\lambda 0} Y_{\lambda 0}(\theta')\right\}$$

PRC 94, 064605 (2016)

$$+ R_{0i}\beta_{20}\left[\frac{\delta\beta_2}{\beta_{20}}\cos\gamma + \cos\gamma - 1\right]Y_{20}(\theta') + R_{0i}(\beta_{20}+\delta\beta_2)\frac{\sin\gamma}{\sqrt{2}}[Y_{22}(\theta',\varphi') + Y_{2-2}(\theta',\varphi')]$$

$$+ R_{0i}\beta_3\cos\eta Y_{30}(\theta') + R_{0i}\beta_3\frac{\sin\eta}{\sqrt{2}}[Y_{32}(\theta',\varphi') + Y_{3-2}(\theta',\varphi')].$$

Prediction of collective levels for ^{54,56,58}Fe

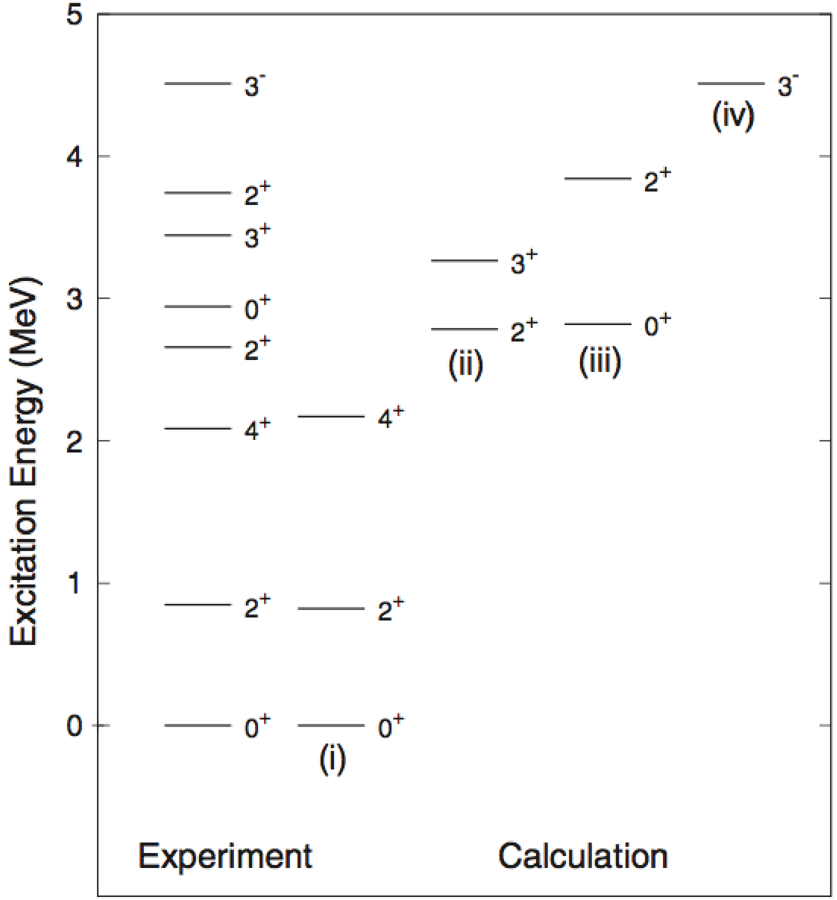


FIG. 1. Comparison of the experimental and predicted level schemes for the ^{56}Fe nucleus.

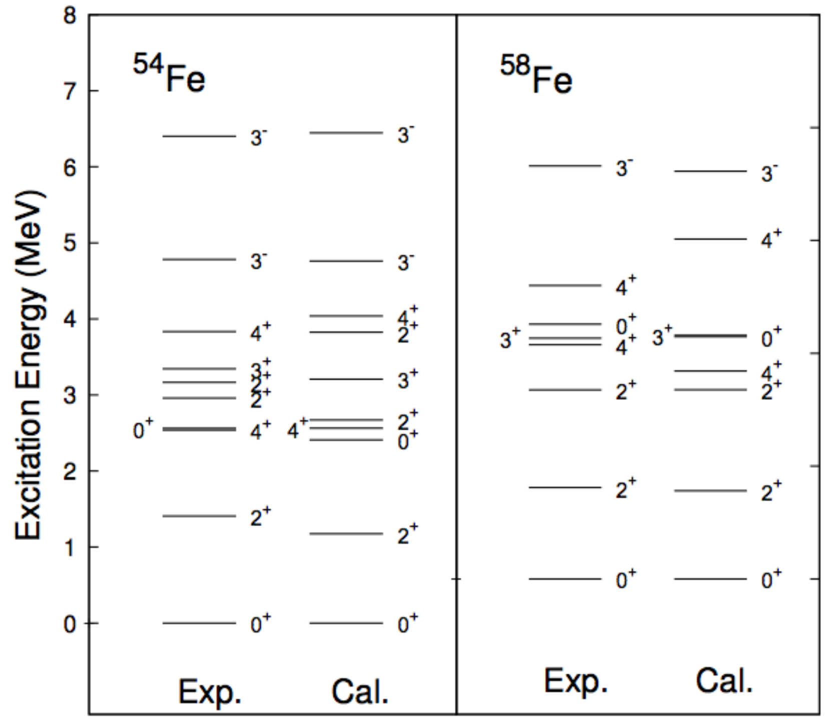
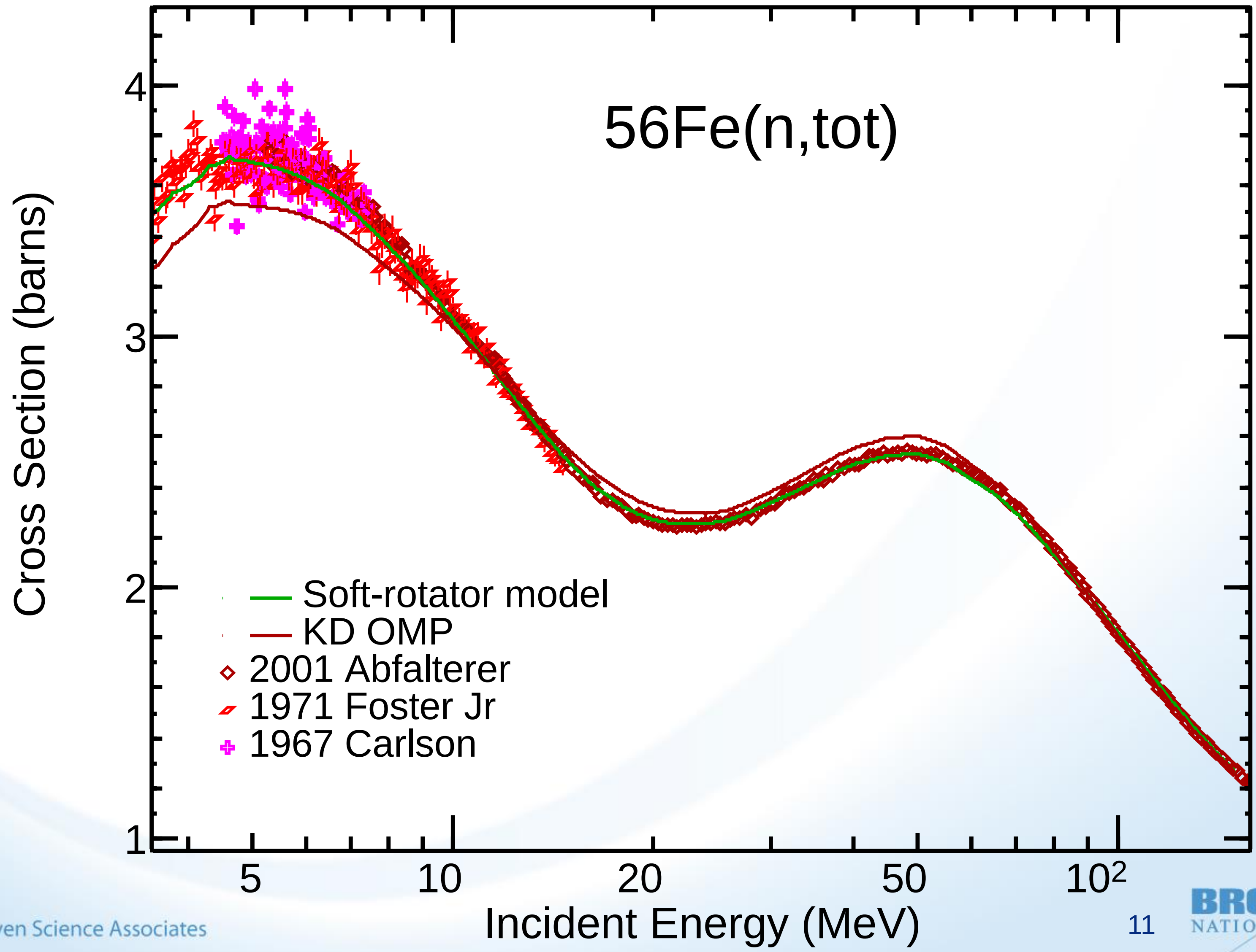


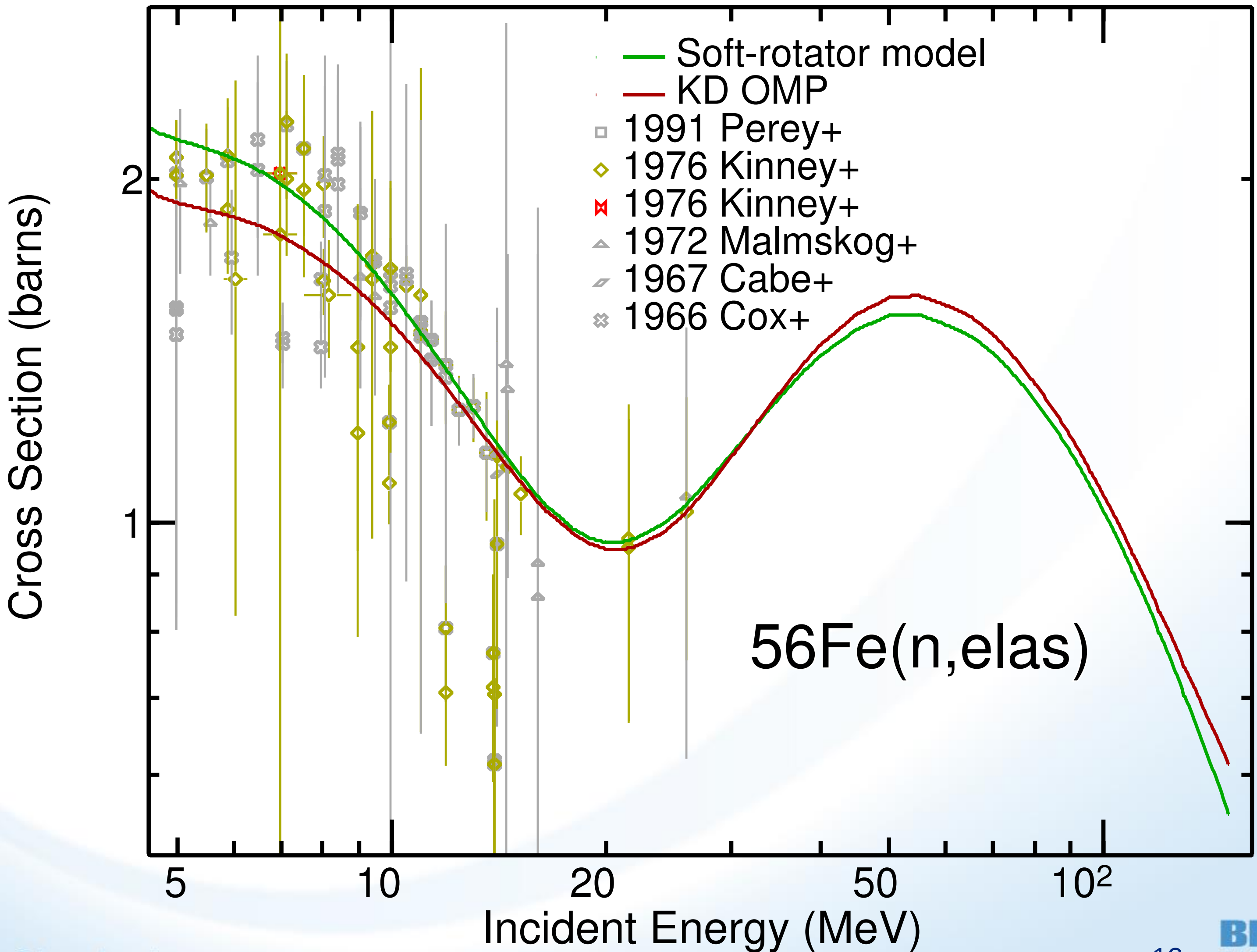
FIG. 1. Comparison of the experimental and SRM predicted collective level schemes for ^{54}Fe and ^{58}Fe nuclei.

PRC 87, 054611 (2013)
NDS 118 (2014) 191-194

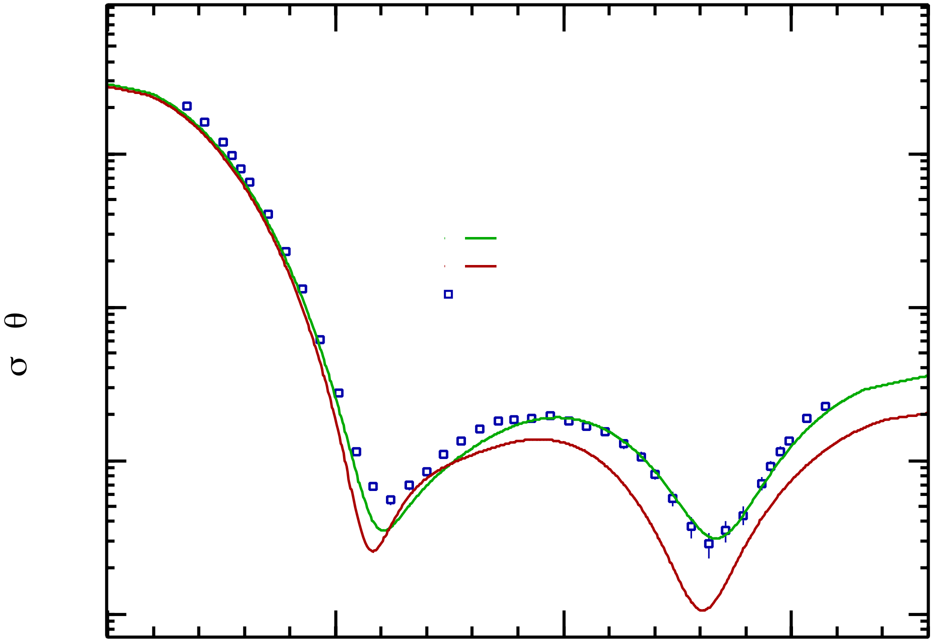
^{56}Fe

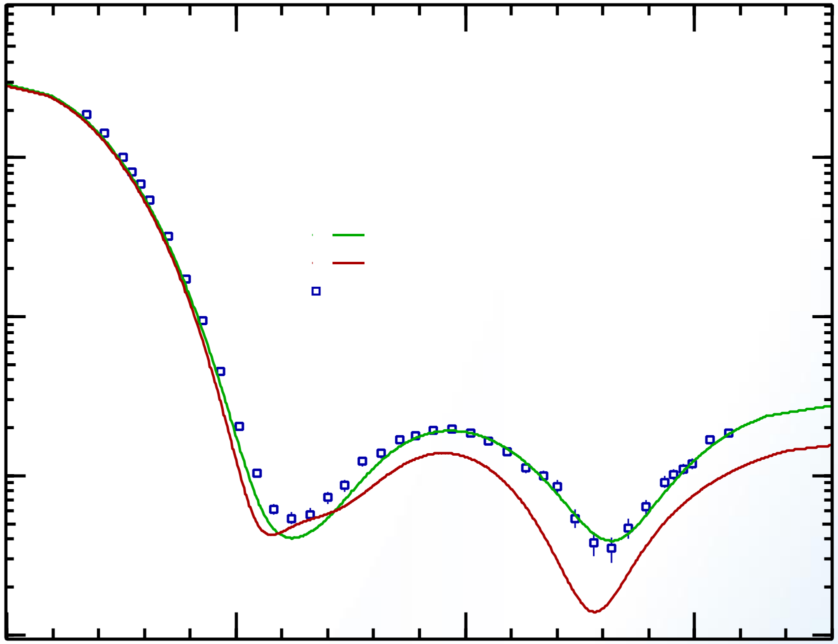

56Fe(n,tot)
Cross Section (barns)
4
3
2
1
Soft-rotator model
KD OMP
2001 Abfalterer
1971 Foster Jr
1967 Carlson
5
10
20
50
10^2
Incident Energy (MeV)

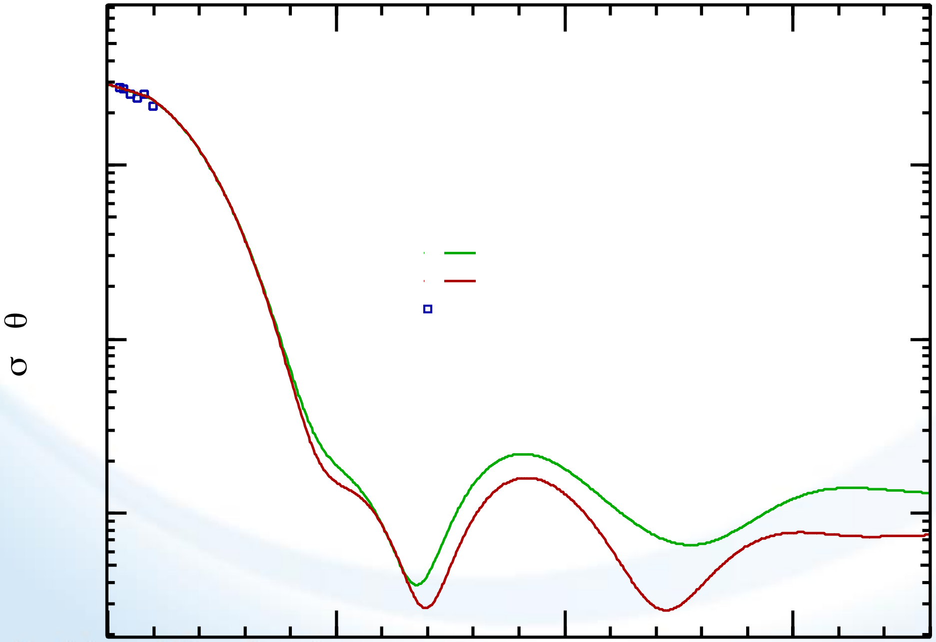
^{56}Fe



Soft-rotator model
KD OMP
1991 Perey+
1976 Kinney+
1976 Kinney+
1972 Malmskog+
1967 Cabe+
1966 Cox+
56Fe(n,elas)
Cross Section (barns)
2
1
5
10
20
50
10^2
Incident Energy (MeV)

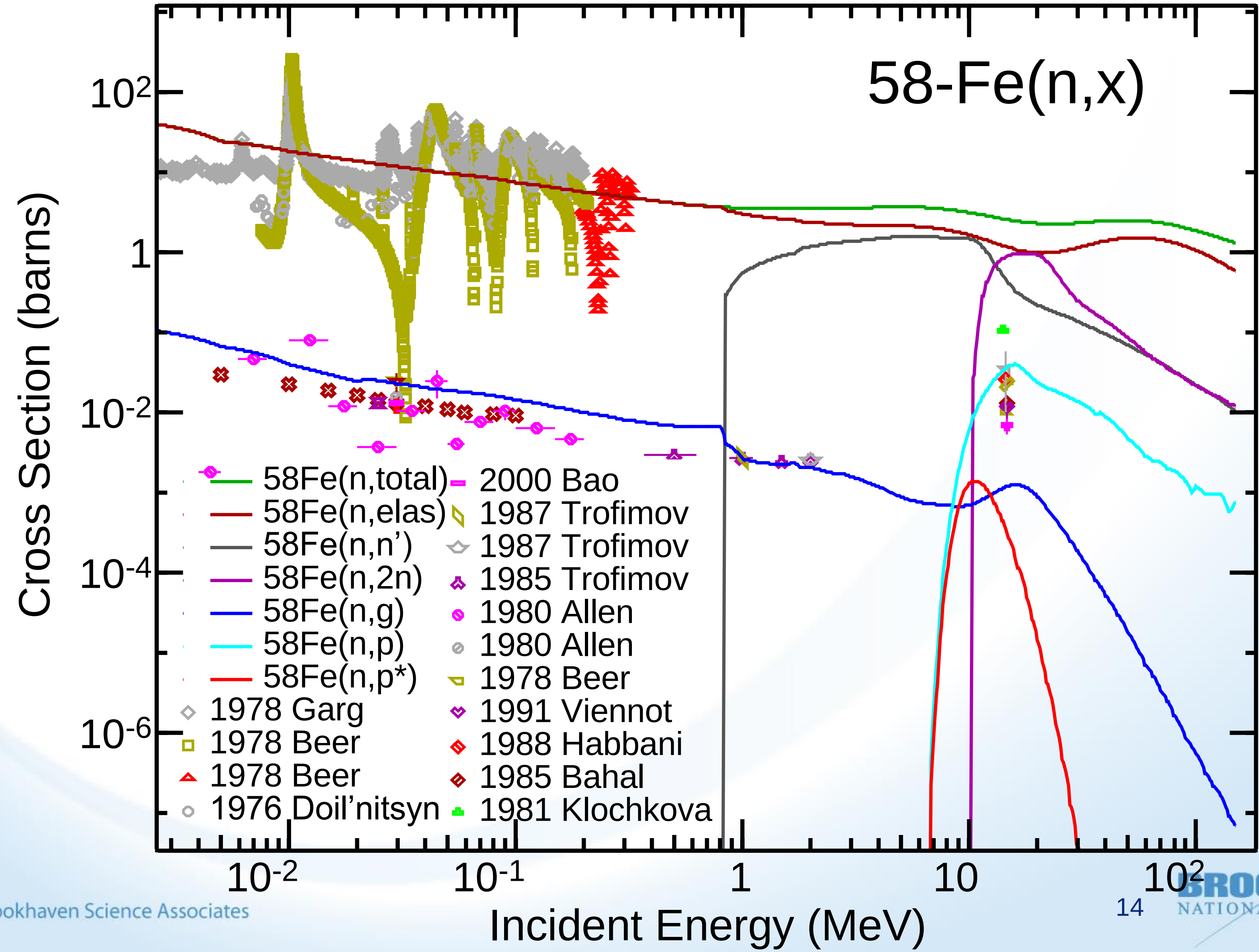






A more fundamental model lends reliability when there is little data available (or none whatsoever).

All data for ^{58}Fe

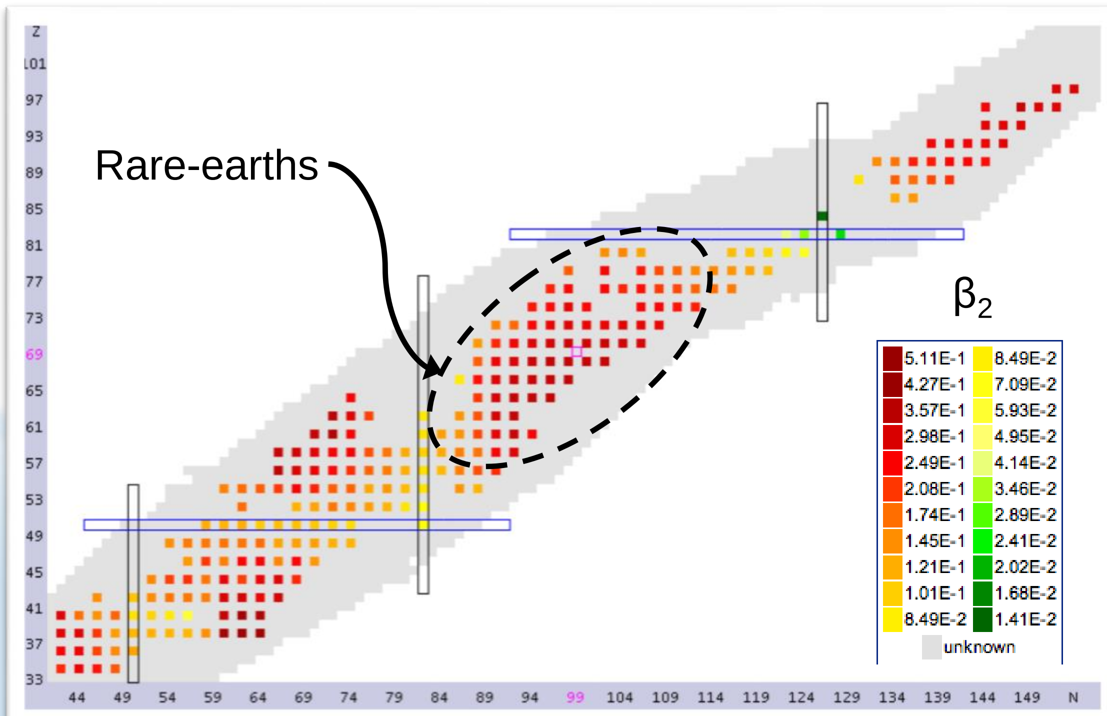


Development of an Optical Model Potential in the rare-earth region

2

Motivation:

- Why seek an optical potential for the rare-earth region?
  - Lack of existing regional OP’s for deformed nuclei
  - Recent work shows scattering from highly deformed nuclei is near adiabatic limit ➔ deforming a spherical global potential may be suitable with only minor modifications



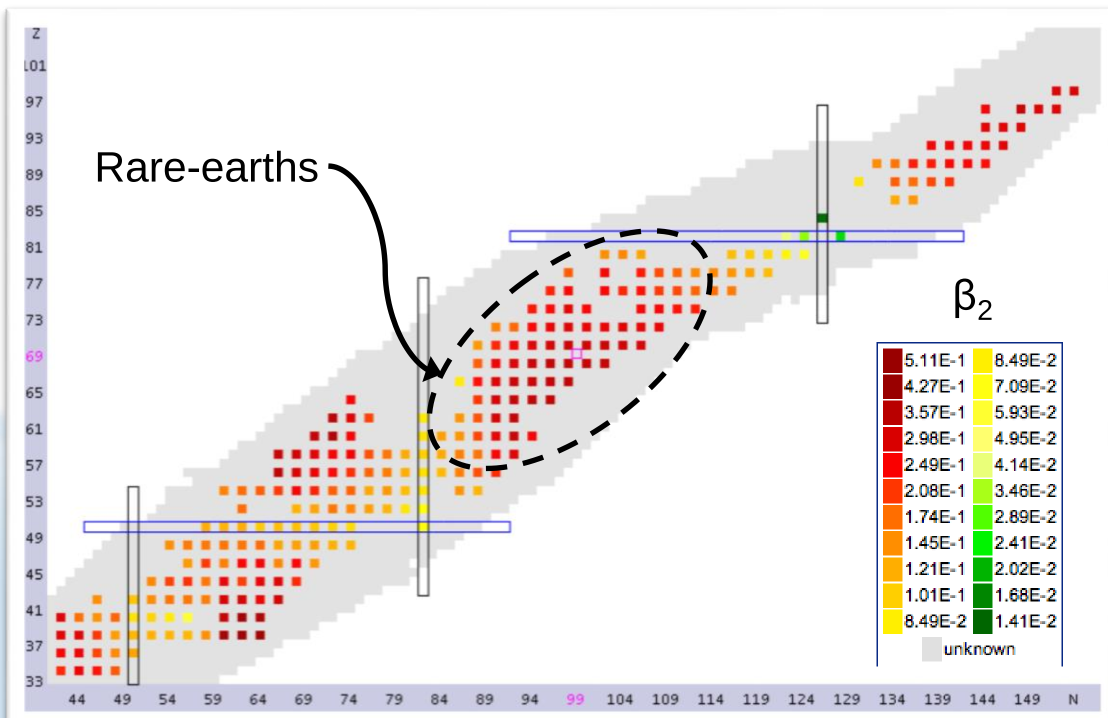
We deform the Koning-Delaroche spherical global potential and couple g.s. rotational band

Development of an Optical Model Potential in the rare-earth region

2

Motivation:

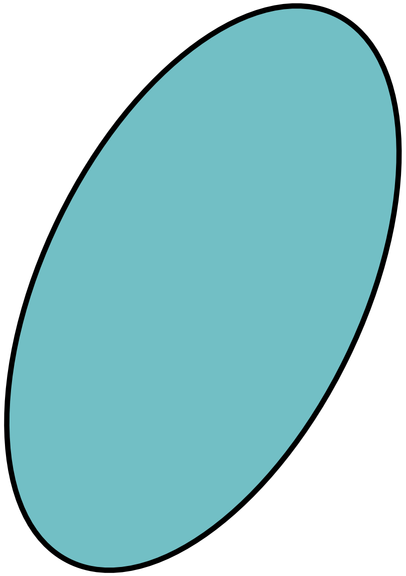
- Why seek an optical potential for the rare-earth region?
  - Lack of existing regional OP's for deformed nuclei
  - Recent work shows scattering from highly deformed nuclei is near adiabatic limit ➔ deforming a spherical global potential may be suitable with only minor modifications



We deform the Koning-Delaroche spherical global potential and couple g.s. rotational band

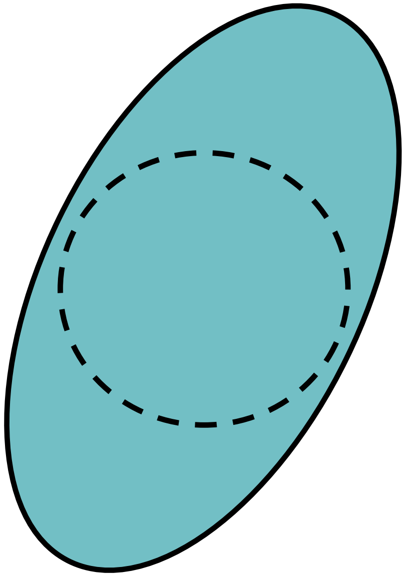
BROOKHAVEN NATIONAL LABORATORY

Very non-rigorous description



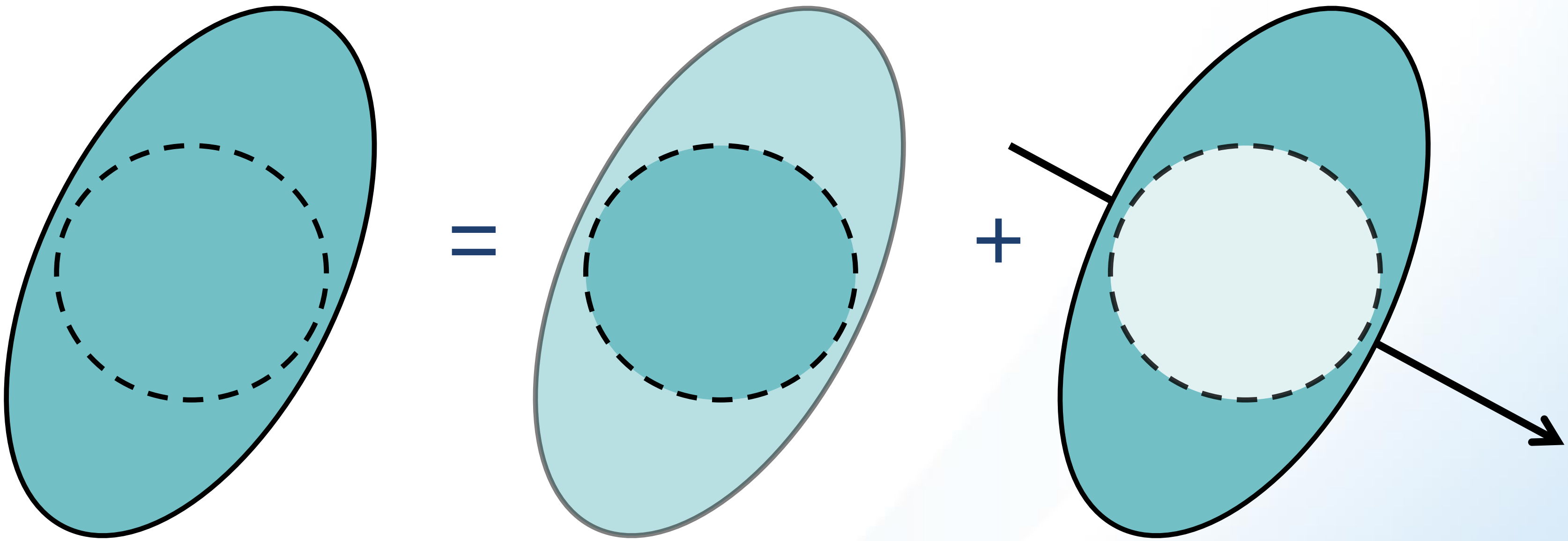
$H_{deformed}$

Very non-rigorous description



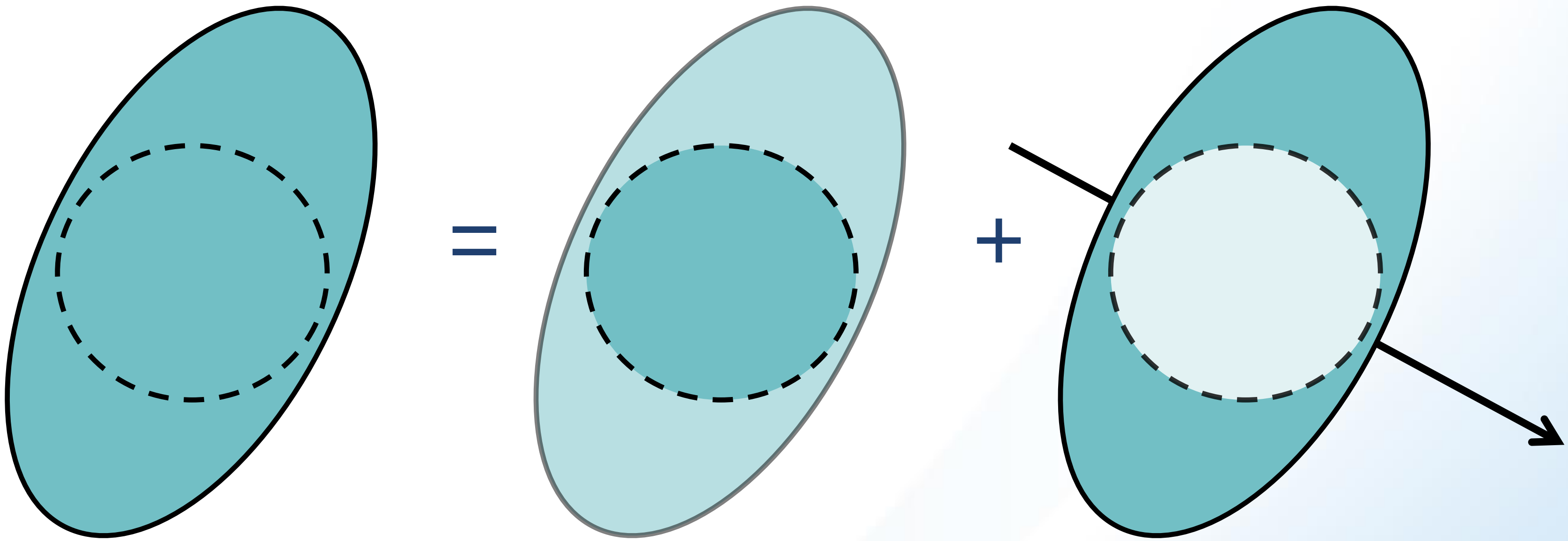
$H_{deformed}$

Very non-rigorous description



$$H_{deformed} = H_{spherical} + H_{rotational}$$

Very non-rigorous description



$$H_{deformed} = \underbrace{H_{spherical}}_{\text{Spher. OMP}} + \underbrace{H_{rotational}}_{\text{CC rot. band}}$$

Calculations done in rare-earths region

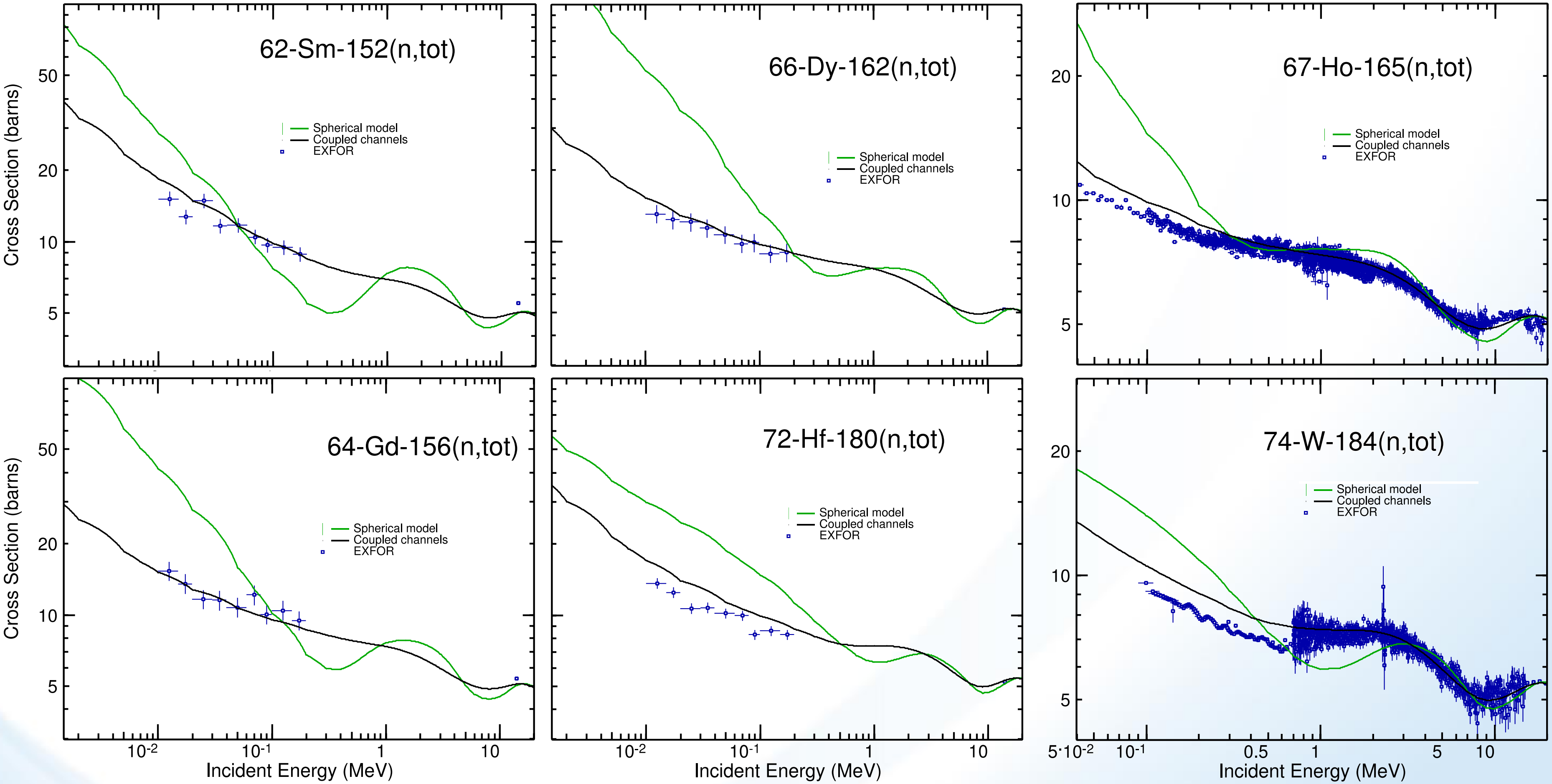
- CC calculations deforming spherical Koning-Delaroche OP
  - Full imaginary part of KD
  - Adiabatic limit
  - Experimental deformations
  - Coupled to g.s. rotational band

$$R(\theta) = R_0 \left(1 + \sum_{\lambda} \beta_\lambda Y_{\lambda,0}(\theta)\right)$$

- Used EMPIRE code (Direct reaction part calculated by ECIS)
- 34 nuclei: ^{162,163,164}Dy, ^{166,167,168,170}Er, ^{153}Eu, ^{155,156,157,158,160}Gd, ^{177,178,179,180}Hf, ^{165}Ho, ^{175,176}Lu, ^{152,154}Sm, ^{181}Ta, ^{159}Tb, ^{169}Tm, ^{182,183,184,186}W, ^{171,172,173,174,176}Yb
- Tested convergence to the number of channels and correction for volume conservation
- Initially compared direct-reaction observables; then extended approach to test effect on compound nucleus quantities

Comparison between spherical and CC:

Total cross sections

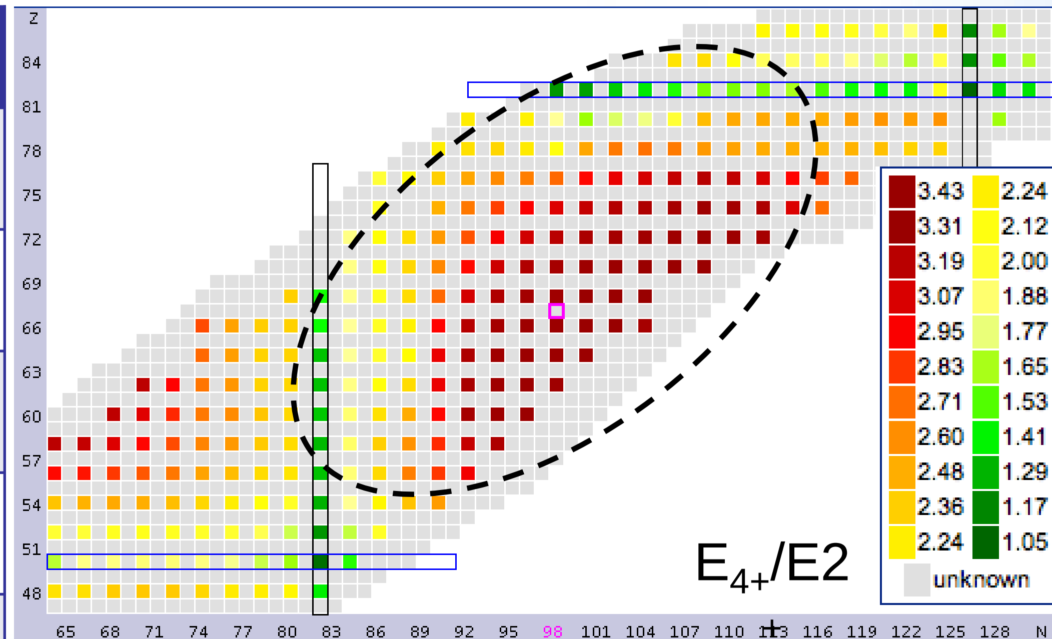


Spherical approach fails at low energy and its shape is often in disagreement with experimental data, while deforming KD potential provides a good description of the observed total cross sections

Angular distributions: Gd, Ho, W

- More detailed analysis on the experimental data sets
- Some elastic ang. dist. data actually contained inelastics
- Ensured convergence regarding number of rotational channels

nucleus	β_2^*	$\beta_4{}^{\S}$	Δ_R	$\beta_2^{(sys)¶}$
^{158}Gd	0.348	0.056	0.990	0.362
^{160}Gd	0.353	0.056	0.990	0.372
^{165}Ho	0.293	-0.020	0.993	0.385
^{182}W	0.251	-0.080	0.995	0.268
^{184}W	0.236	-0.080	0.996	0.255
^{186}W	0.226	-0.080	0.996	0.226



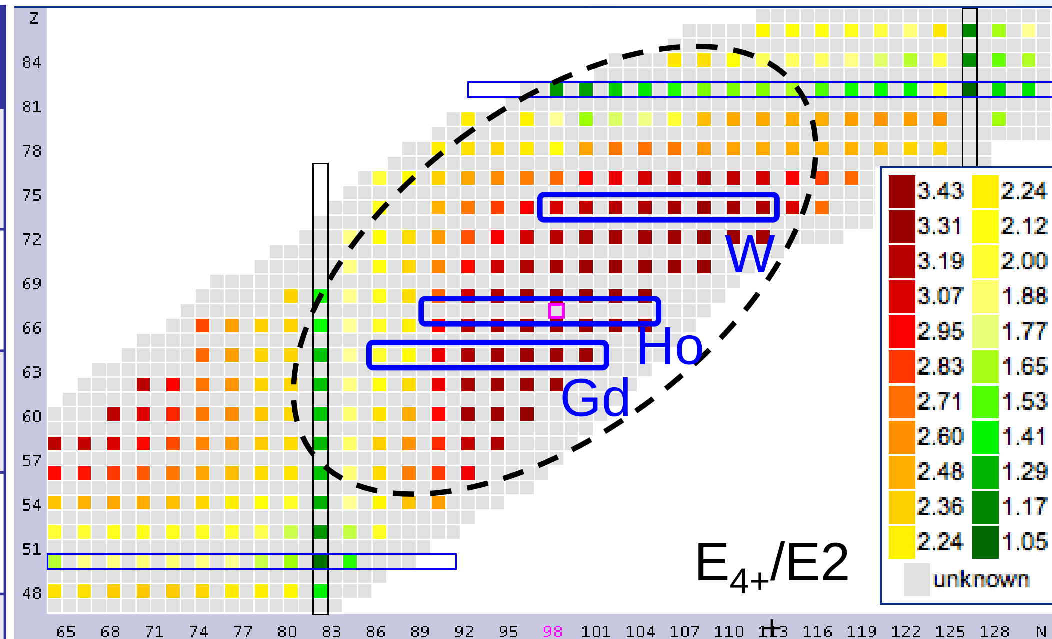
* At. Data. Nucl. & Data Tables, 78, (2001) 1
§ Ann. Nucl. Energy, 31 (2004) 1813; Phys. Lett. 26B (1968) 127; Ann. Nucl. Energy, 28 (2001) 1745

¶ Phys. Rev. C 70 (2004) 014604; Phys. Rev. C 76 (2007) 024605

Angular distributions: Gd, Ho, W

- More detailed analysis on the experimental data sets
- Some elastic ang. dist. data actually contained inelastics
- Ensured convergence regarding number of rotational channels

nucleus	β_2^*	$\beta_4{}^{\S}$	Δ_R	$\beta_2^{(sys)\P}$
^{158}Gd	0.348	0.056	0.990	0.362
^{160}Gd	0.353	0.056	0.990	0.372
^{165}Ho	0.293	-0.020	0.993	0.385
^{182}W	0.251	-0.080	0.995	0.268
^{184}W	0.236	-0.080	0.996	0.255
^{186}W	0.226	-0.080	0.996	0.226

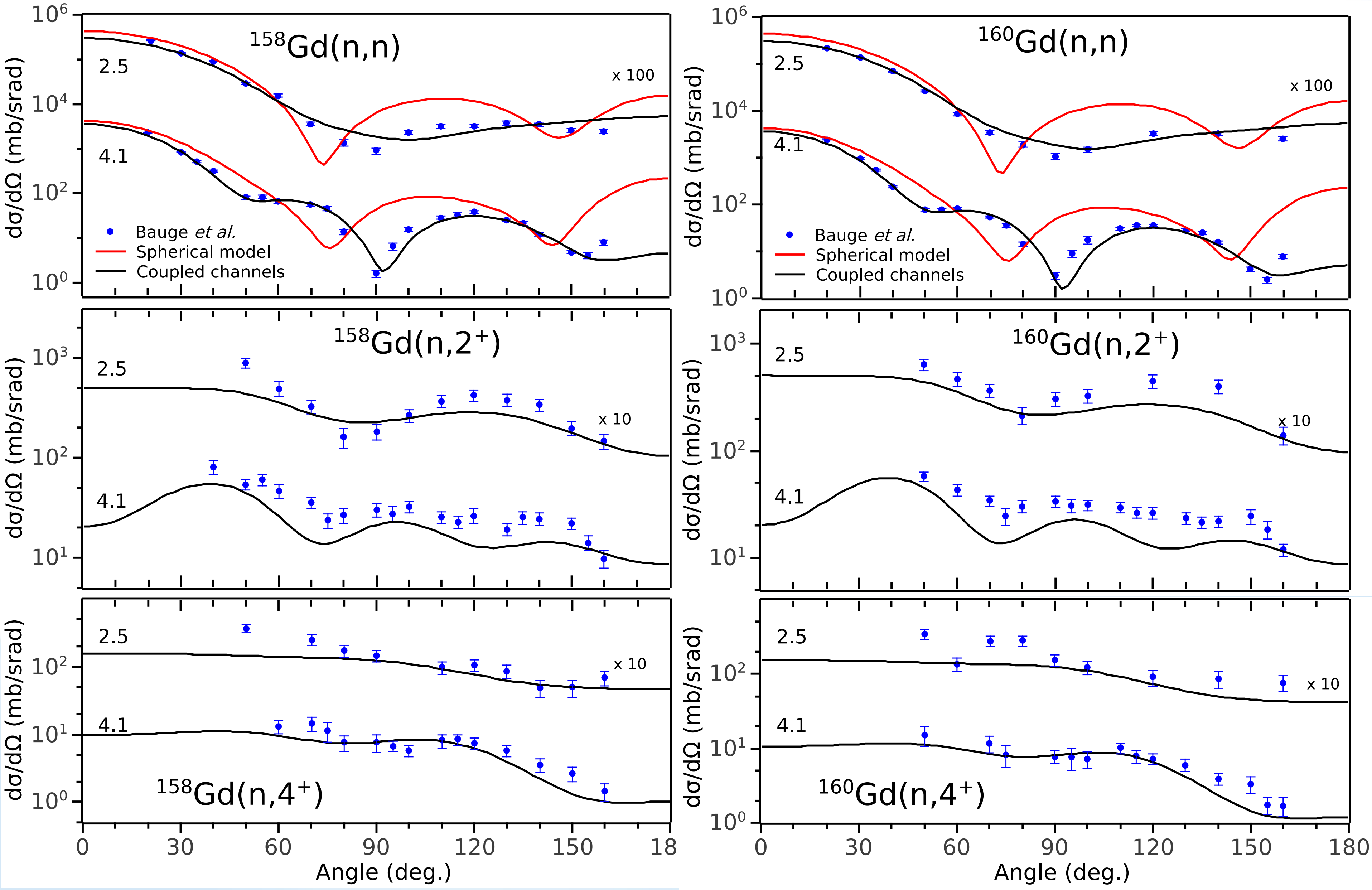


* At. Data. Nucl. & Data Tables, 78, (2001) 1
§ Ann. Nucl. Energy, 31 (2004) 1813;
Phys. Lett. 26B (1968) 127;
Ann. Nucl. Energy, 28 (2001) 1745

¶ Phys. Rev. C 70 (2004) 014604;
Phys. Rev. C 76 (2007) 024605

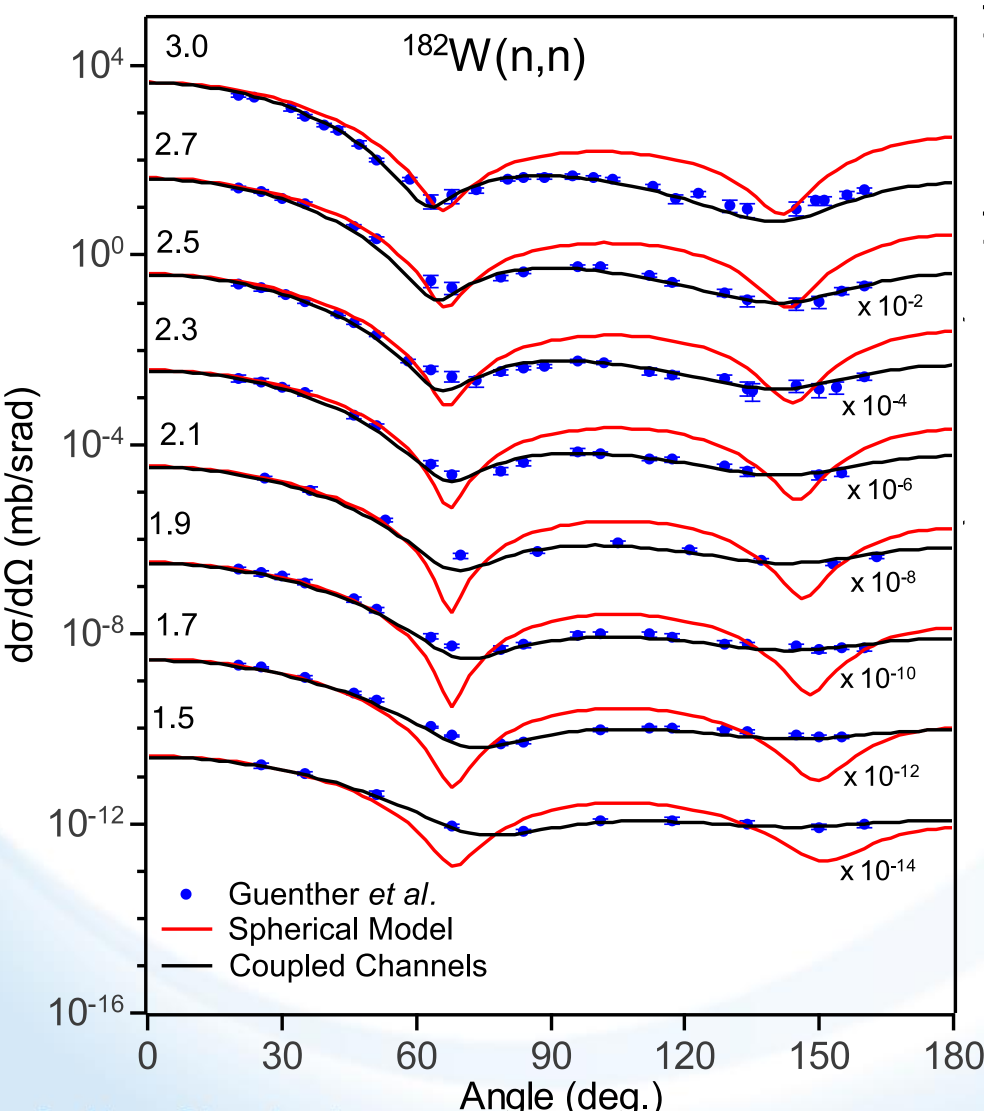
$^{158, 160}$Gd Angular distributions

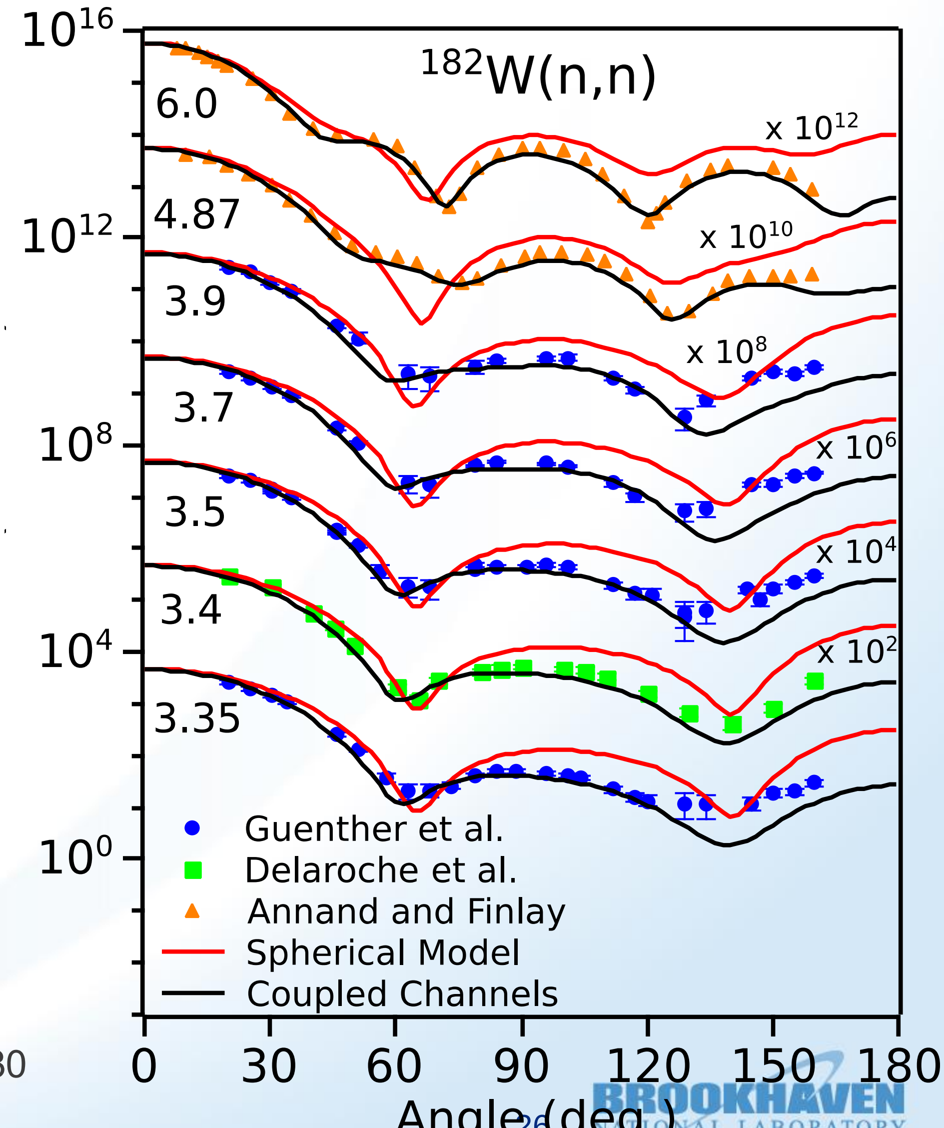
Good agreement with experimental data obtained by the model



^{182}W – Elastic angular distributions

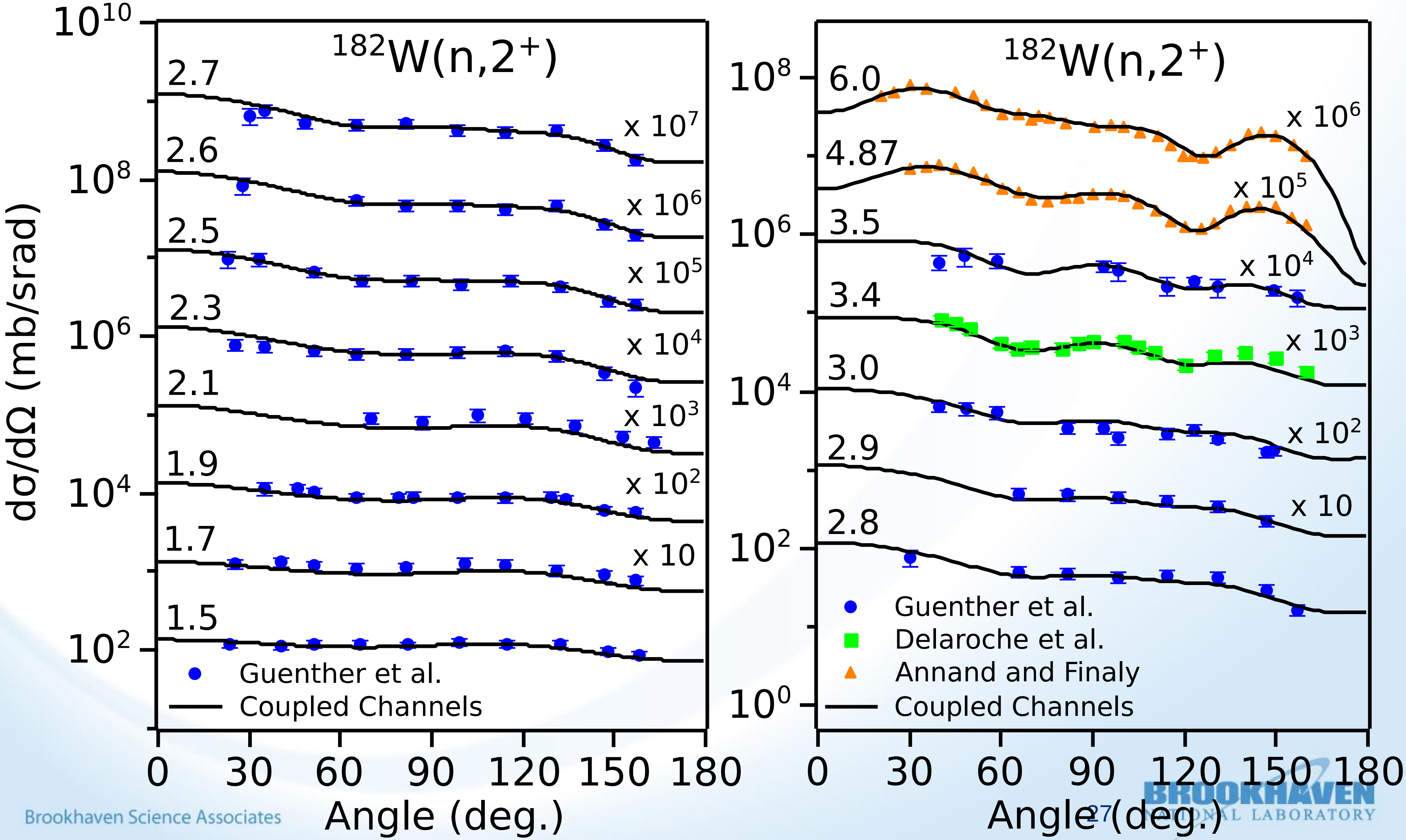
Good agreement with experimental data obtained by the model





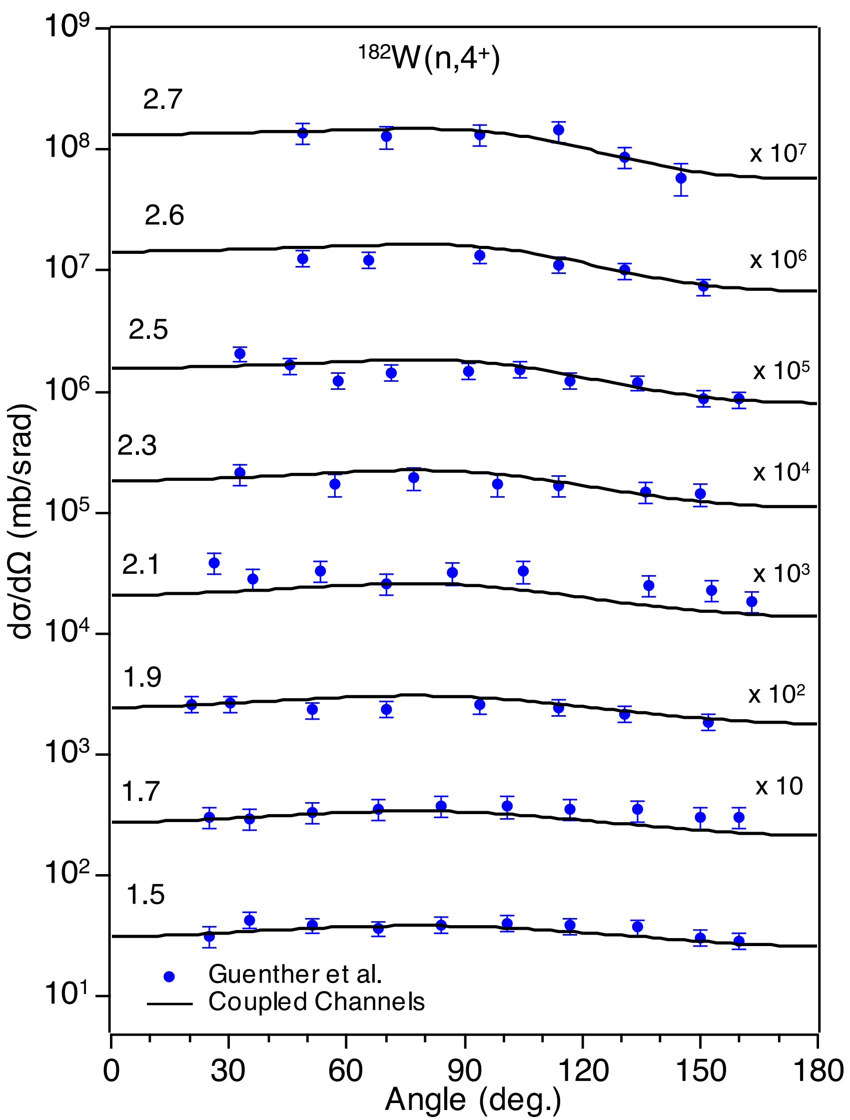
^{182}W – 2^{+} Inelastic ang. dist. (E_{2^+}=0.100MeV)

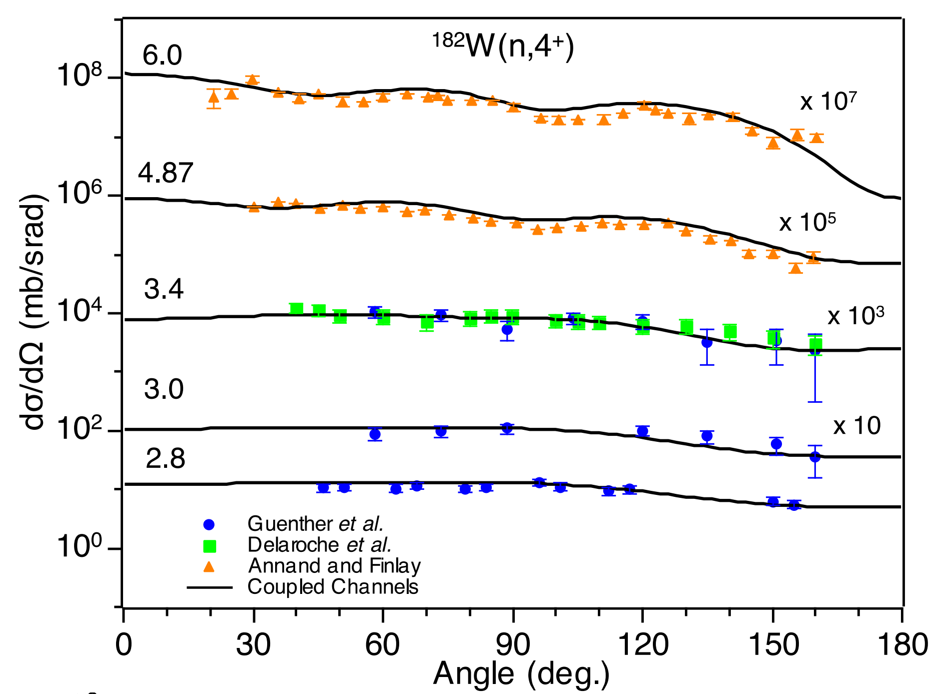
Good agreement with experimental data obtained by the model

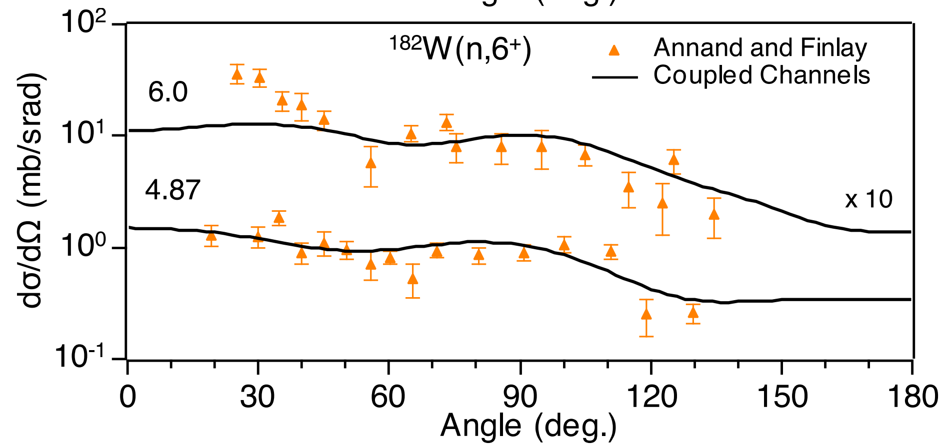


^{182}W – 4^+ Inelastic ang. dist. (E_{4^+}=0.329MeV)

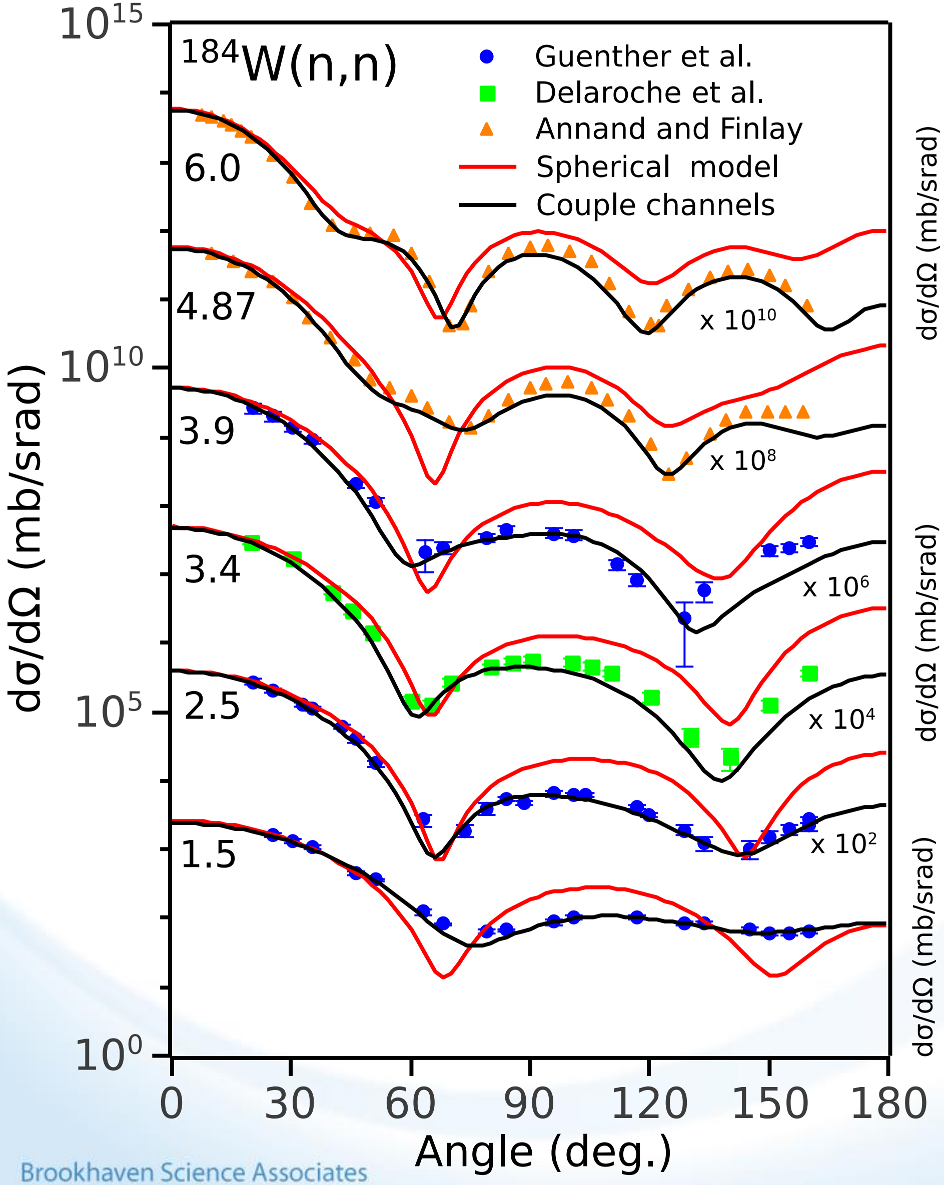
Good agreement with experimental data obtained by the model

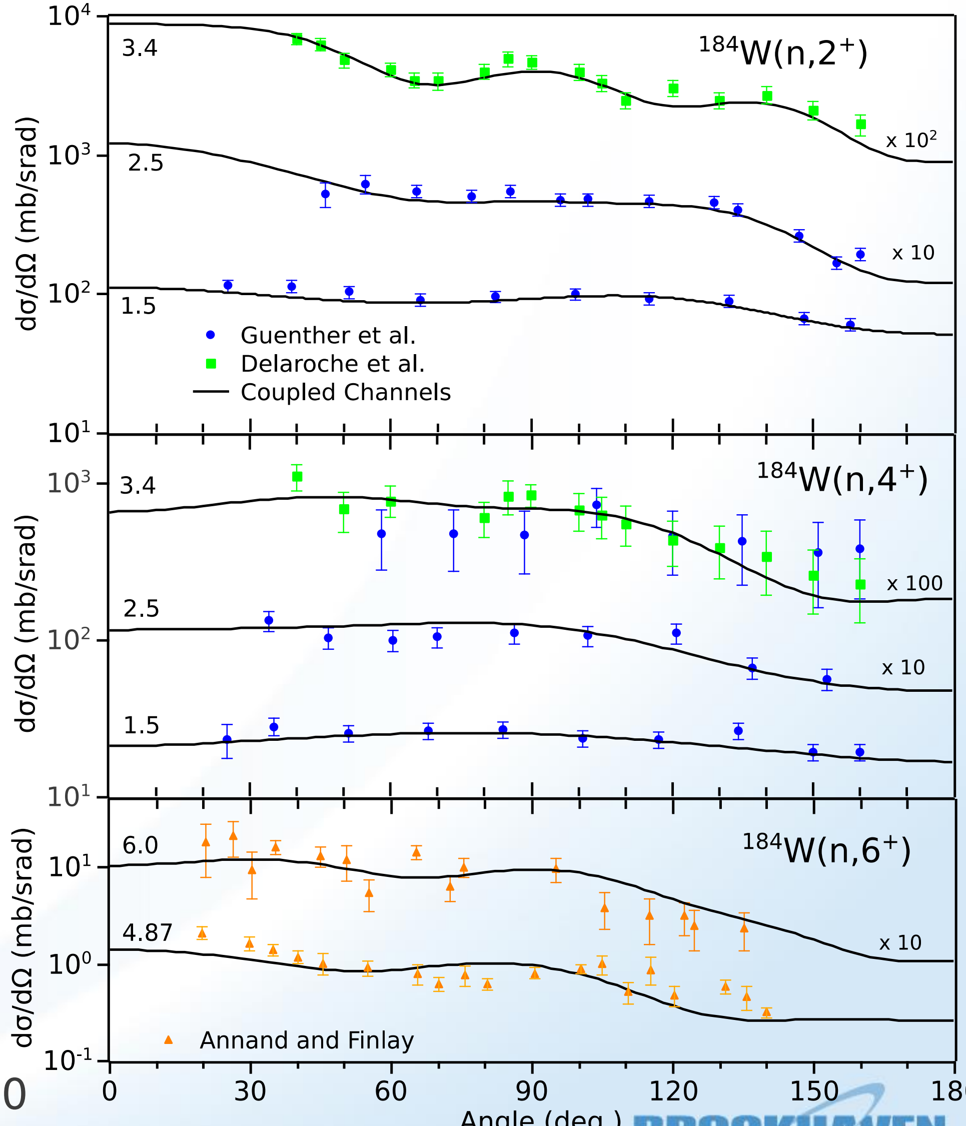




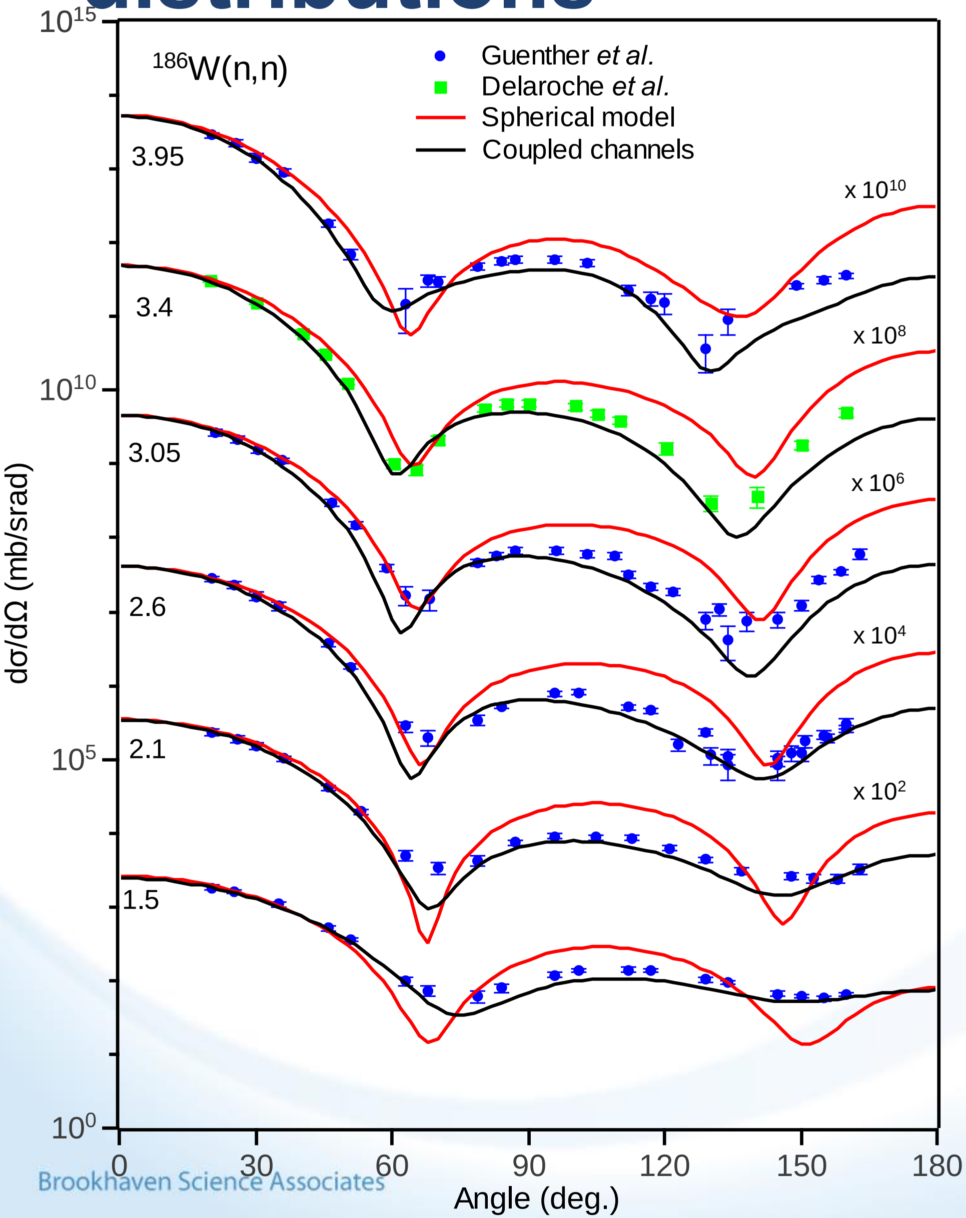


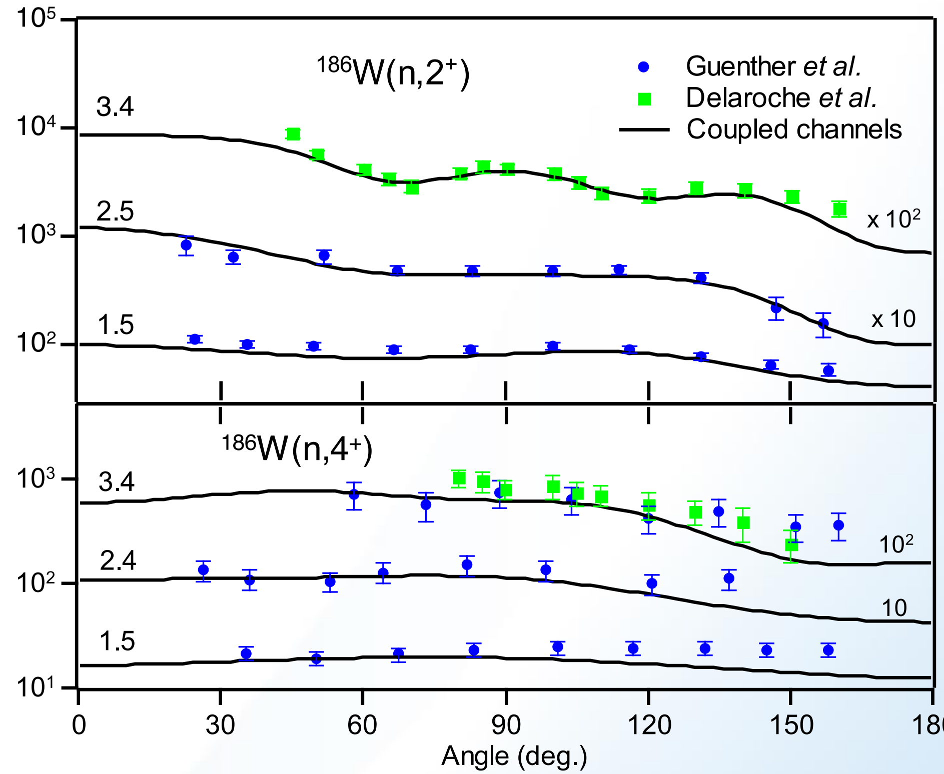
^{184}W – Elastic and inelastic angular distributions





^{186}W – Elastic and inelastic angular distributions





The fact that deforming KD allows to consistently describe observed elastic and inelastic angular distributions remarkably well is very supportive of the model and of the adiabatic approximation.

Reaction observables from Energy Density Functionals

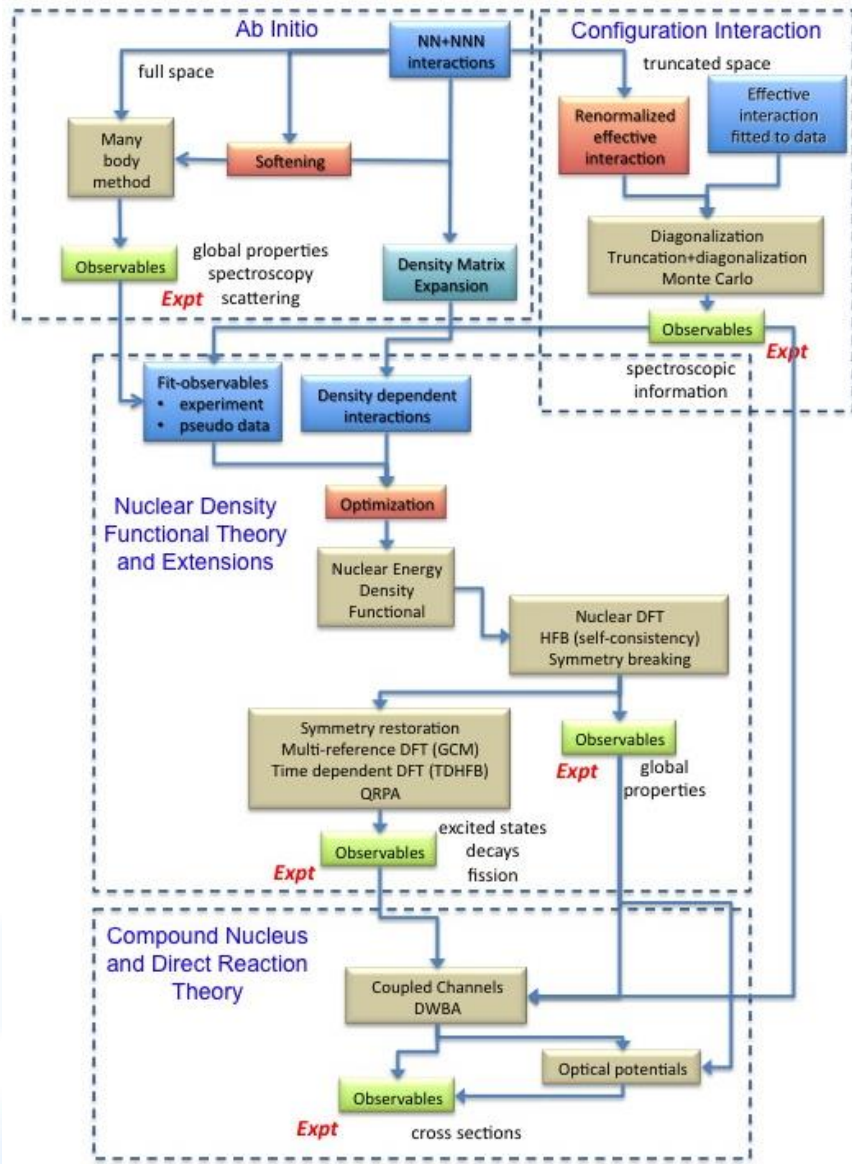
3

UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

Main goals:

- To find an optimal energy density functional (EDF) using all our knowledge of the nucleonic Hamiltonian and basic nuclear properties.
- To apply the EDF theory and its extensions to validate the functional using all the available relevant nuclear structure data.
- To apply the validated theory to properties of interest that cannot be measured, in particular the transition properties needed for reaction theory.



Reaction observables from Energy Density Functionals

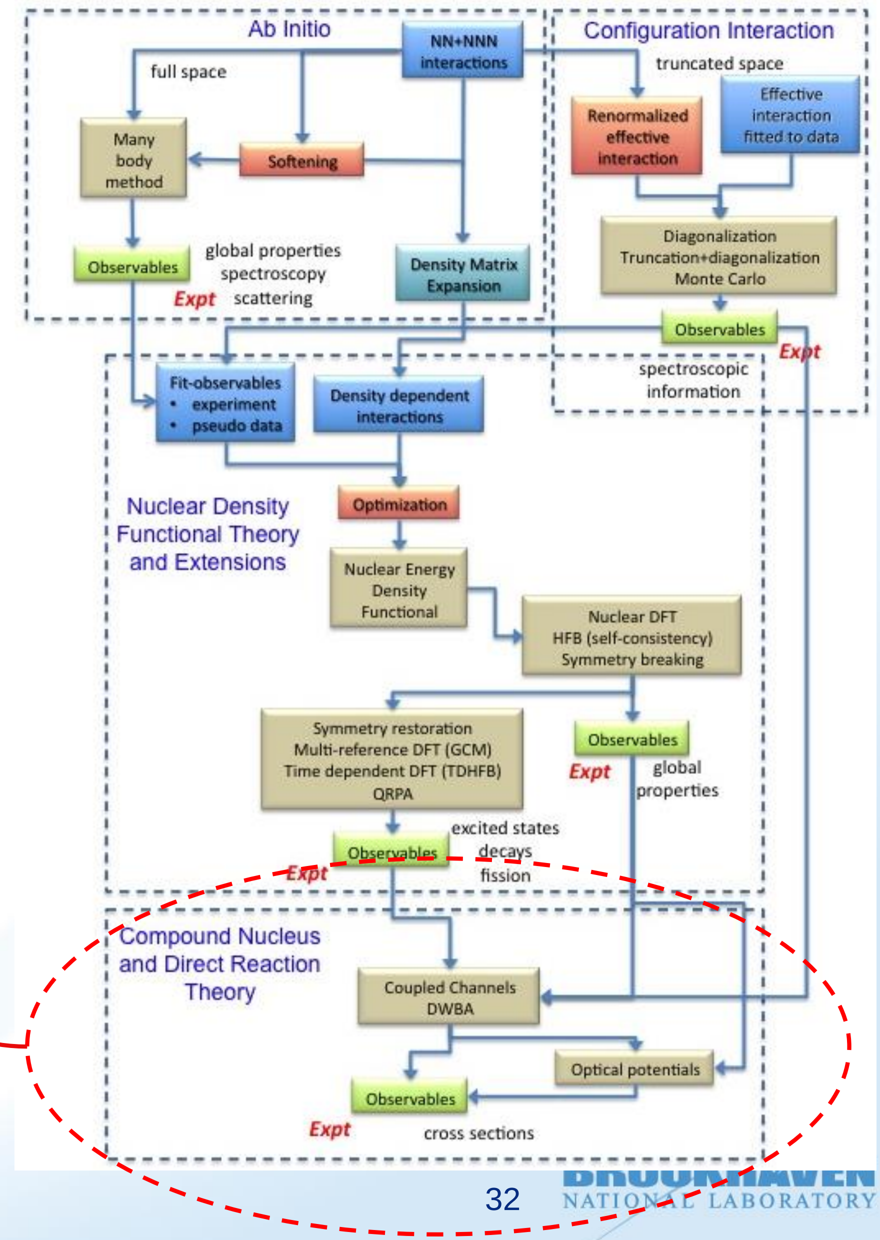
3

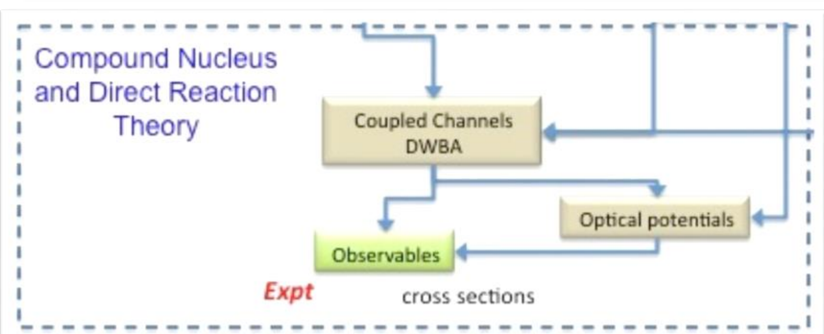
UNEDF SciDAC Collaboration

Universal Nuclear Energy Density Functional

Main goals:

- To find an optimal energy density functional (EDF) using all our knowledge of the nucleonic Hamiltonian and basic nuclear properties.
- To apply the EDF theory and its extensions to validate the functional using all the available relevant nuclear structure data.
- To apply the validated theory to properties of interest that cannot be measured, in particular the transition properties needed for reaction theory.



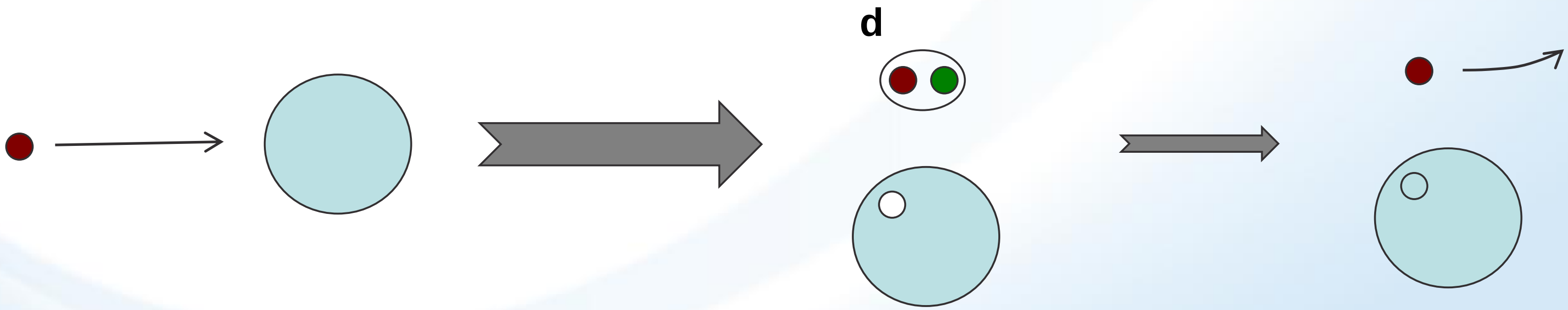


Outline of Coupled-Channels Calculations

- Mean-field HFB calculations using SLy4 Skryme functional
- Use (Q)RPA to find all levels E*, with transition densities from the g.s.
- Structure calculations for n,p + ^{40,48}Ca, ^{58}Ni, ^{90}Zr and ^{144}Sm
- Fold transition densities with effective n-n interaction: Transition Potentials
- Couple to all excited states, E* < 10, 20, 30, 40 MeV
- Find what fraction of σ_R corresponds to inelastic couplings: more states, larger σ_R, until all open channels are coupled
- Couple to all pickup channels leading to deuteron formation

Outline of Coupled-Channels Calculations

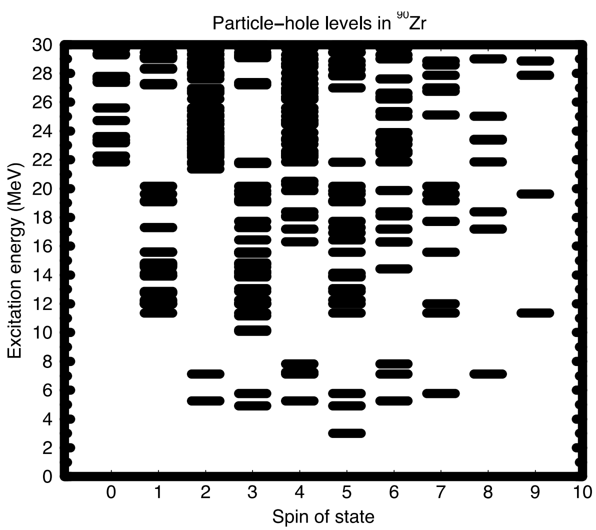
- Mean-field HFB calculations using SLy4 Skryme functional
- Use (Q)RPA to find all levels E*, with transition densities from the g.s.
- Structure calculations for n,p + ^{40,48}Ca, ^{58}Ni, ^{90}Zr and ^{144}Sm
- Fold transition densities with effective n-n interaction: Transition Potentials
- Couple to all excited states, E* < 10, 20, 30, 40 MeV
- Find what fraction of σ_R corresponds to inelastic couplings: more states, larger σ_R, until all open channels are coupled
- Couple to all pickup channels leading to deuteron formation



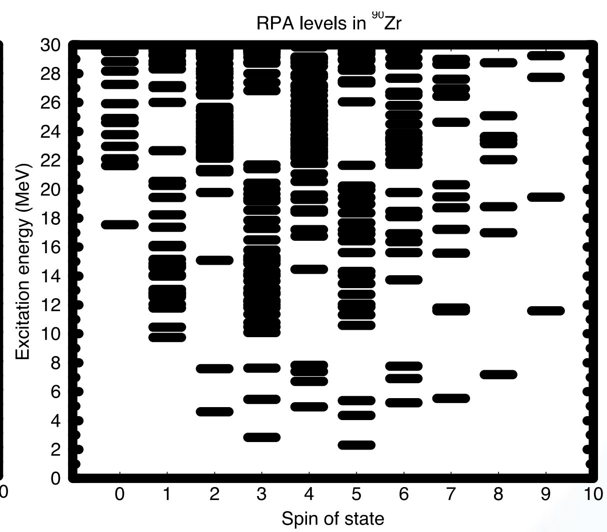
Nuclear Excited States from Mean-field Models

- Mean-field HFB calculations using SLy4 Skryme functional
- Use (Q)RPA to find all levels E*, with transition densities from the g.s.

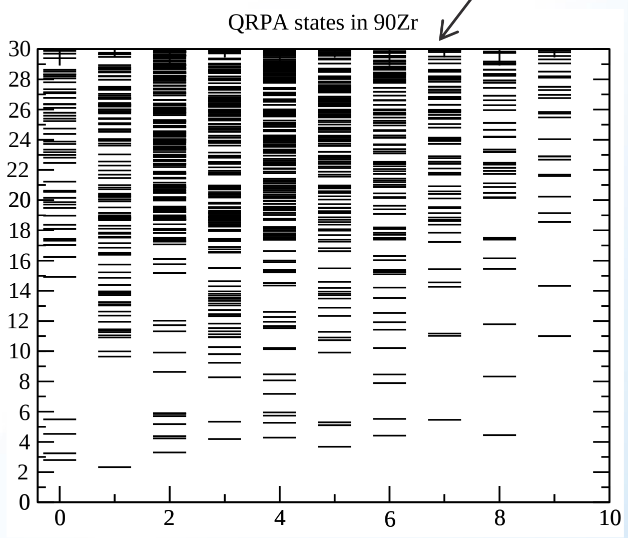
Collaboration with Chapel Hill: Engel & Terasaki



Uncorrelated particle-hole states



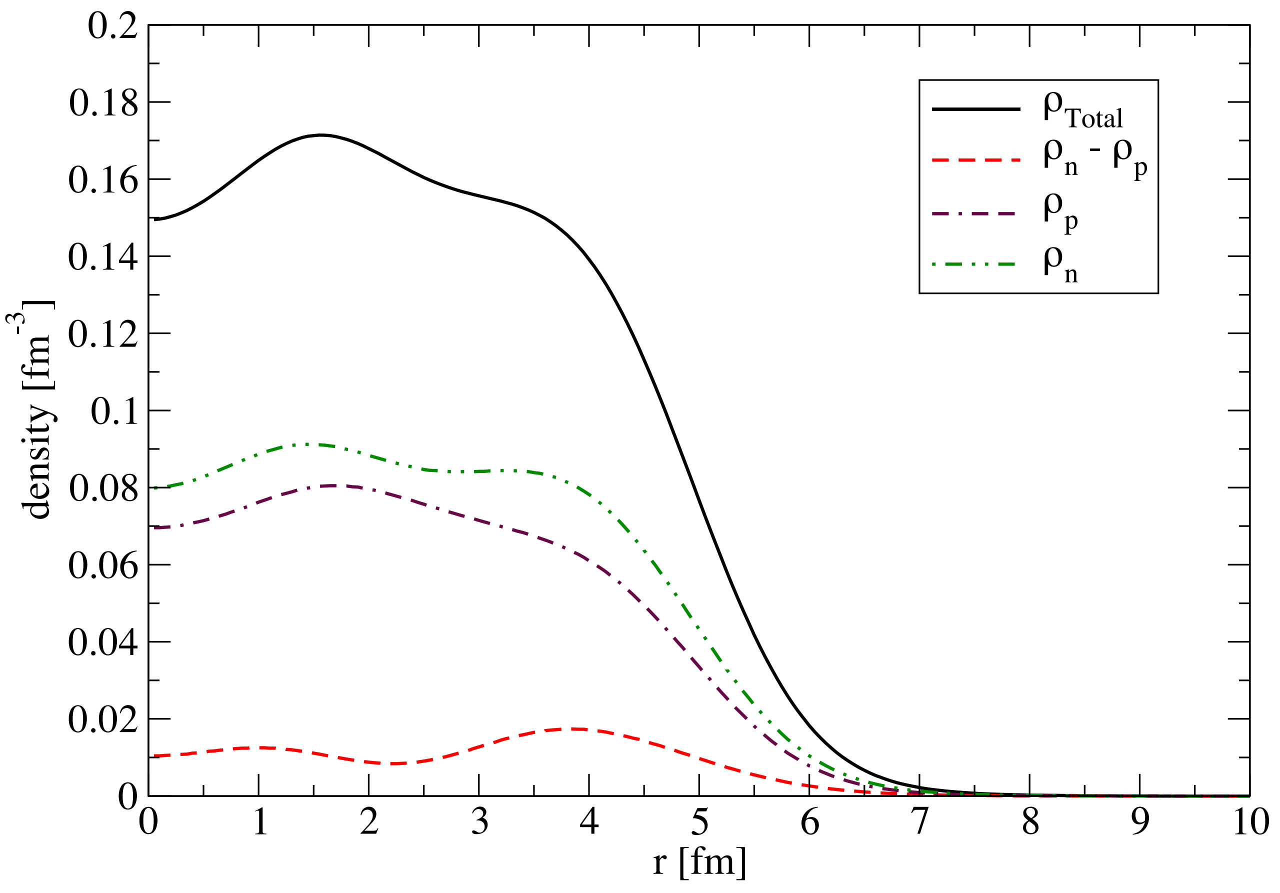
Correlated p-h states in HO basis



Correlated p-h states in 15 fm box

Neutron separation energy is 9.5 MeV.
Above this we have discretized continuum.

Diagonal Density



Example of diagonal Density for ^{90}Zr

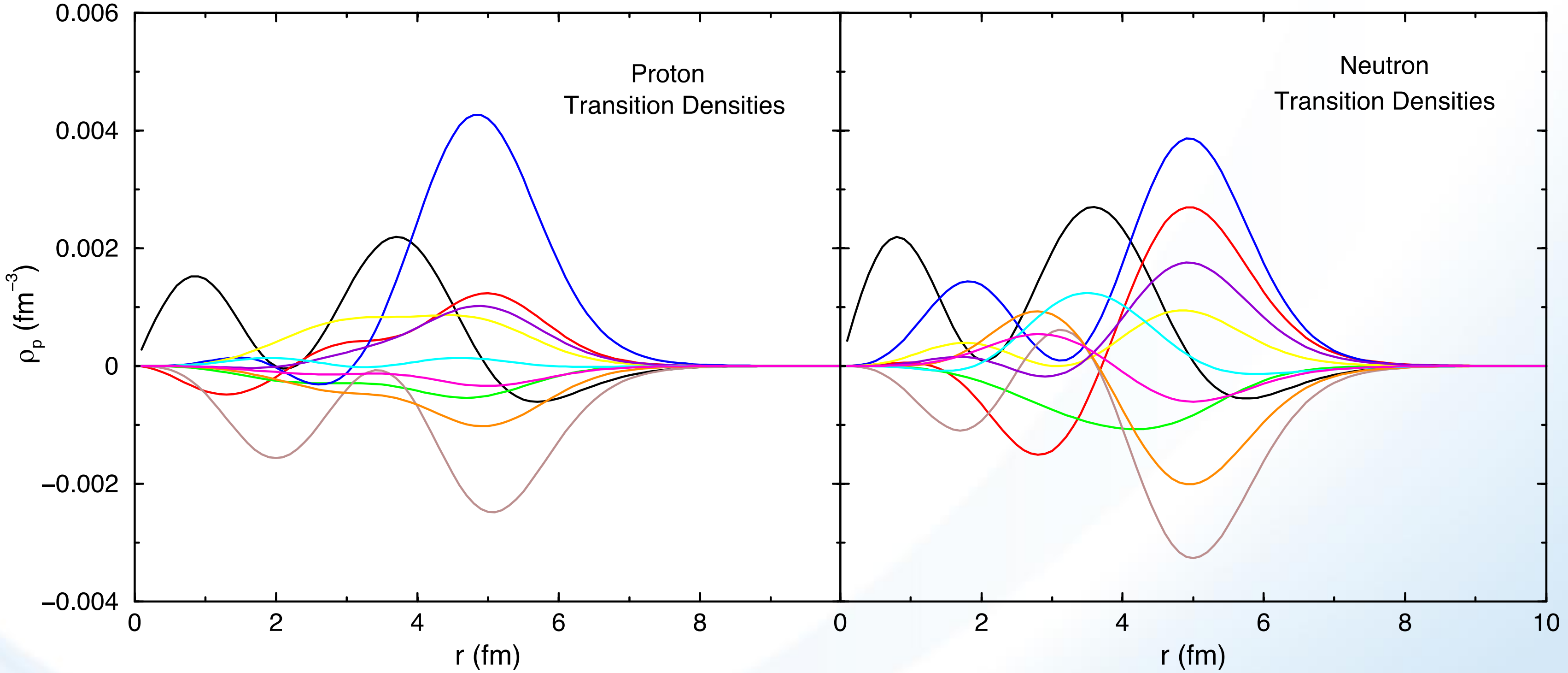
RPA

Folding of densities with n-n interaction Transition potentials

Off-Diagonal Densities

Example of off- diagonal Transition densities for ^{90}Zr

RPA
$E^* < 10$ MeV; $J^{\pi}_{max} = 4^+$

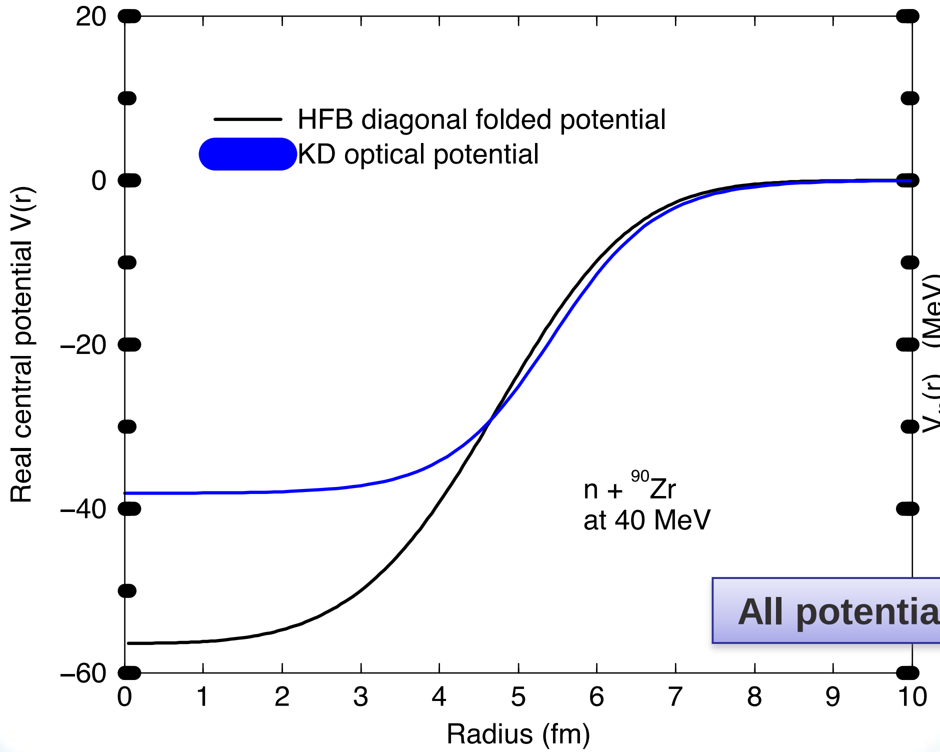


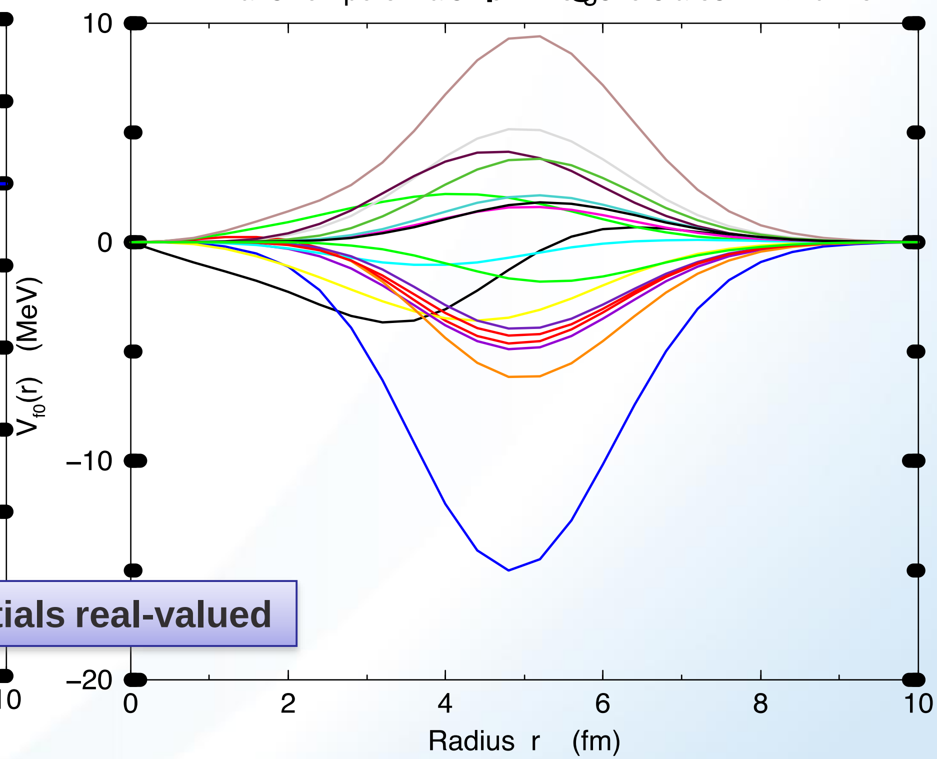
Folding of densities with n-n interaction □ Transition potentials

Transition densities to Transition potentials

Diagonal folded potential

Off-diagonal couplings



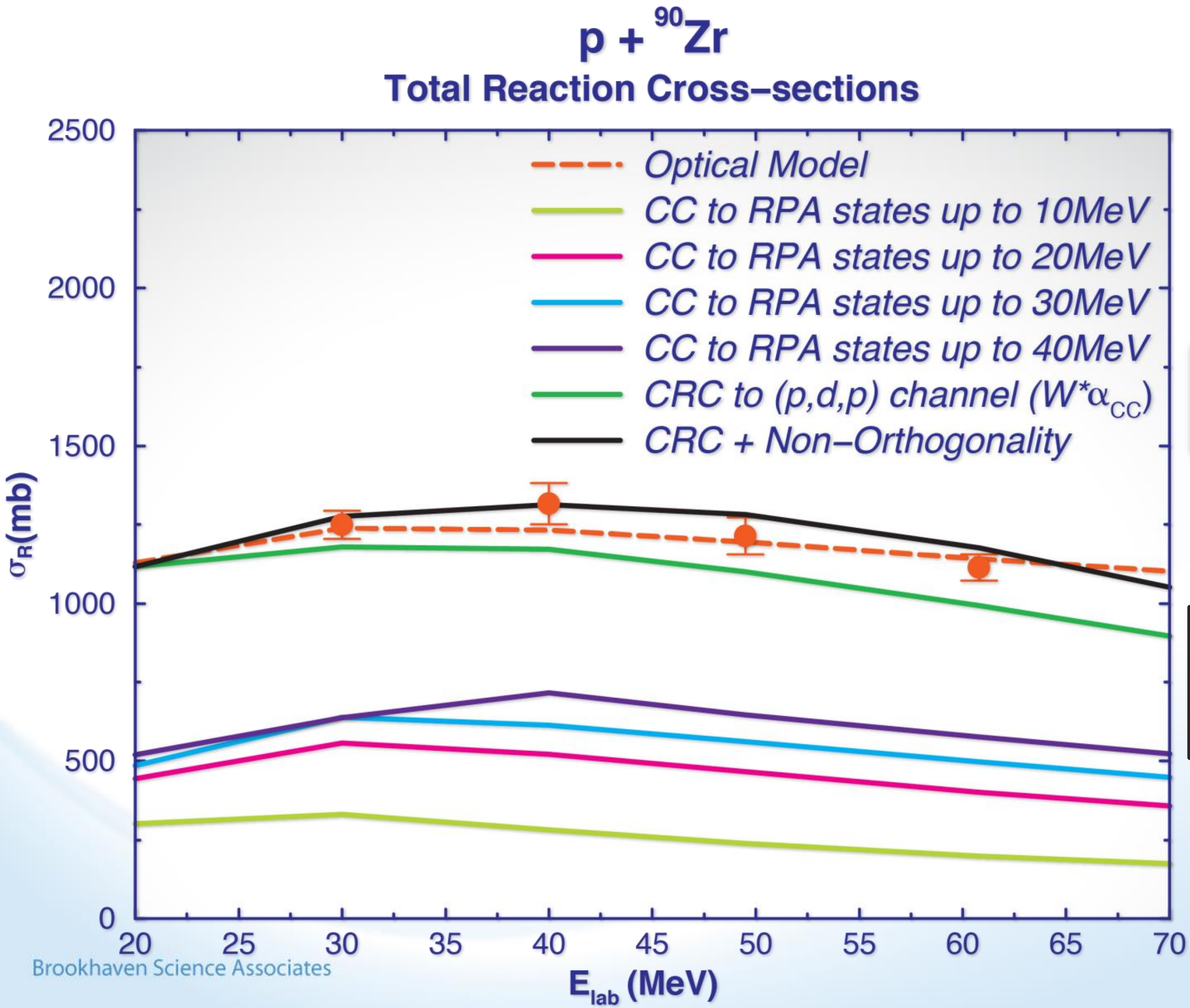


All potentials real-valued

Natural parity states only: no spin-flip, so no spin-orbit forces generated.
No energy or density dependence. Exchange contributions included implicitly.

(So far…)

Comparison with Experimental Data

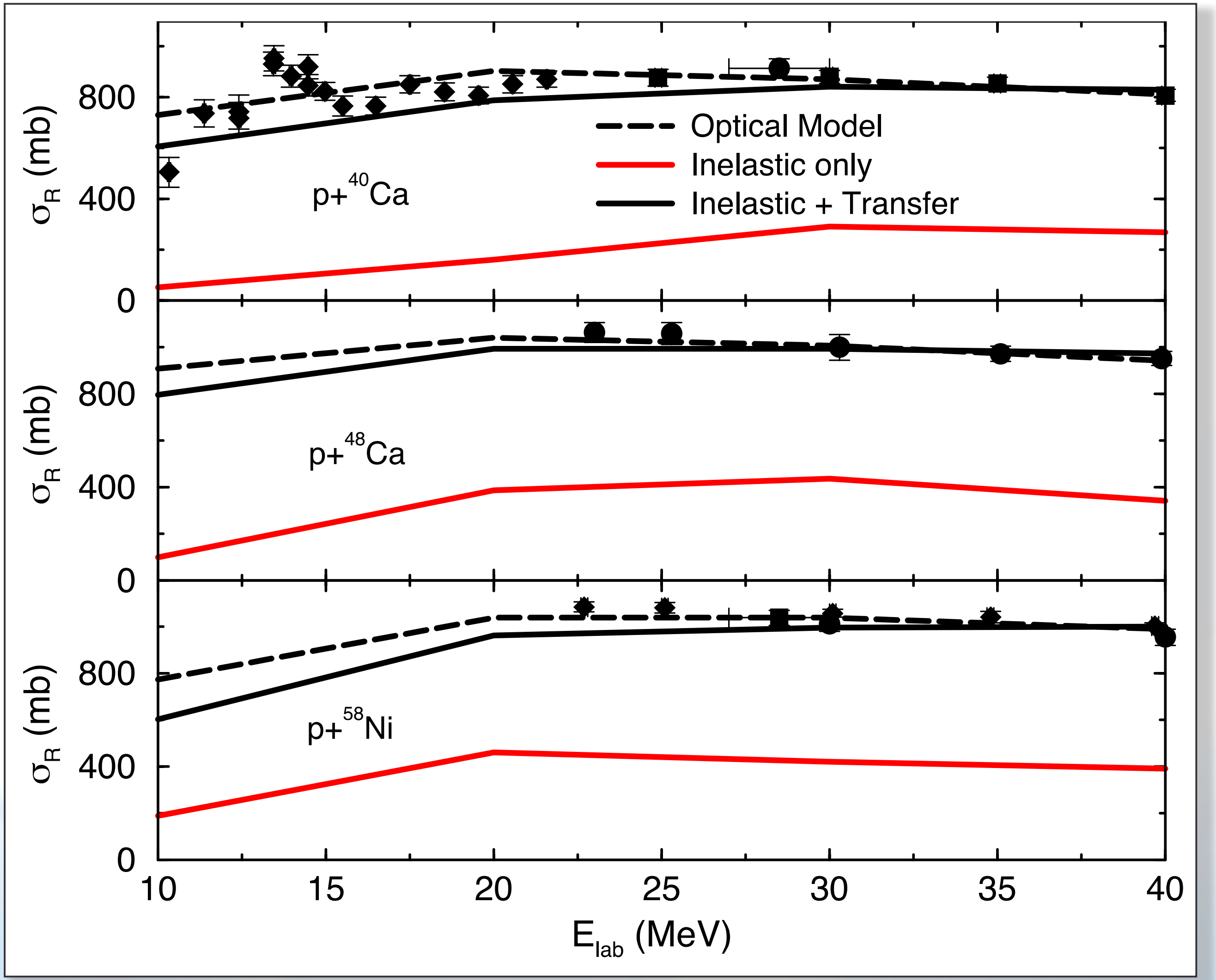


Inelastic convergence when coupling up to all open channels

Good description of experimental data!

Inelastic and pick-up channels account for all reaction cross sections

Comparison with Experimental Data



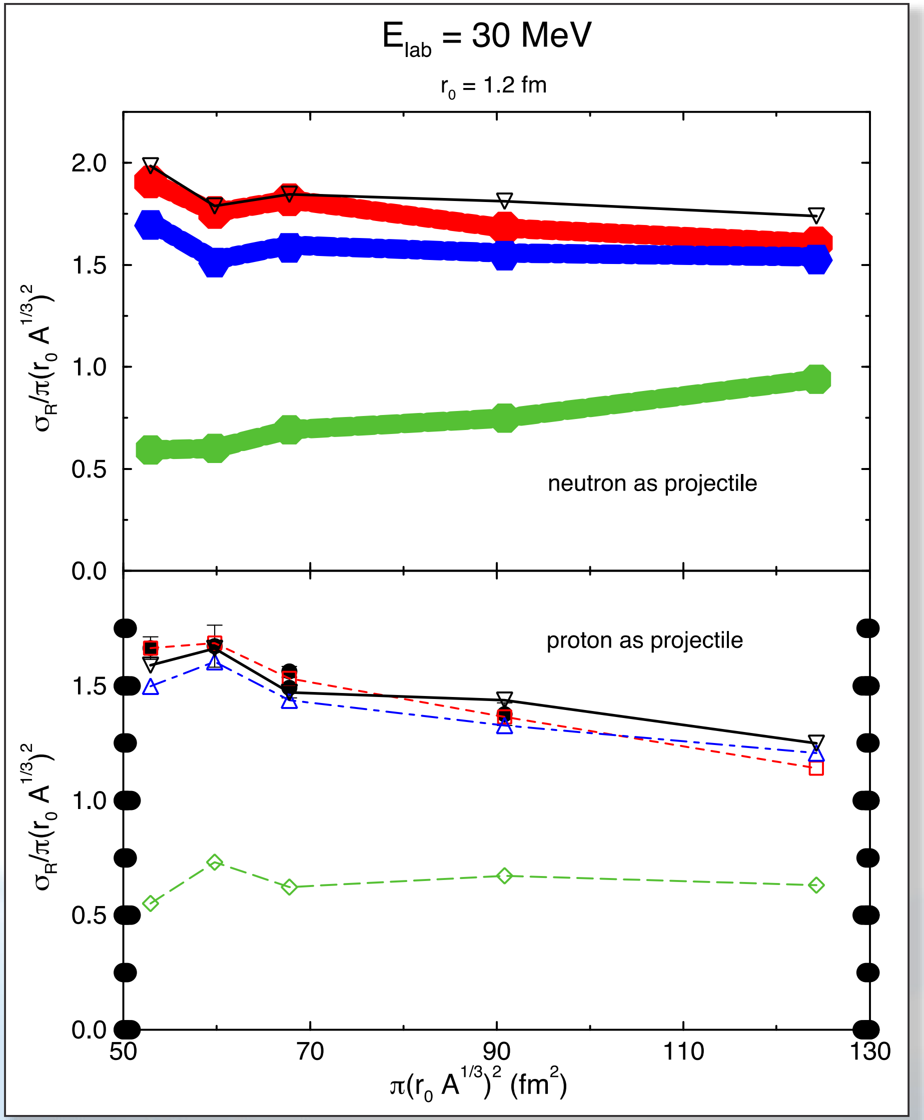
Good description of experimental data!

Inelastic and pick-up channels account for all reaction cross sections

G. P. A. Nobre, F.S. Dietrich, J. E. Escher, I. J. Thompson, M. Dupuis, J. Terasaki and J. Engel

Phys. Rev. Lett. 105, 202502 (2010)

Summary of Results at E_{lab} = 30 MeV



Targets

^{40}Ca, ^{48}Ca, ^{58}Ni, ^{90}Zr, ^{144}Sm

- Phenomenological Optical Model
- Inelastic couplings only
- Inelastic + Transfer
- Inelastic + Transfer with non-orthogonality

With all couplings, calculations agree with experimental data

Phys. Rev. Lett. 105, 202502 (2010)
Phys. Rev. C 84, 064609 (2011)

G. P. A. Nobre, F.S. Dietrich, J. E. Escher, I. J. Thompson, M. Dupuis, J. Terasaki and J. Engel

Two-Step Approximation

We found we need only two-step contributions

- These simply add for all j=1,N inelastic & transfer states:

$$V_{DPP} = \Sigma_j^N \; V_{0j} \;\; G_j \;\; V_{j0}.$$

$G_j = [E_n - e_j - H_j]^{-1}$: channel-j Green's function

$V_{j0} = V_{0j}$: coupling form elastic channel to excited state j

- Gives $V_{DPP}(r,r',L,E_n)$: nonlocal, L- and E-dependent.

In detail: $V_{DPP}(r,r',L,E_n) = \Sigma_j^N \; V_{0j}(r) \;\; G_{jL}(r,r') \;\; V_{j0}(r') = V + iW$

- Quadratic in the effective interactions in the couplings V_{ij}
- Can be generalized to non-local $V_{ij}(r,r')$ more easily than CCh.
- Treat any higher-order couplings as a perturbative correction

Tried by Coulter & Satchler (1977), but only some inelastic states included

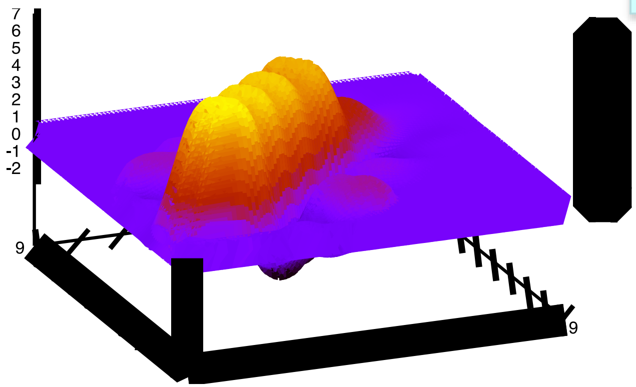
Calculated Nonlocal Potentials V(r,r') now

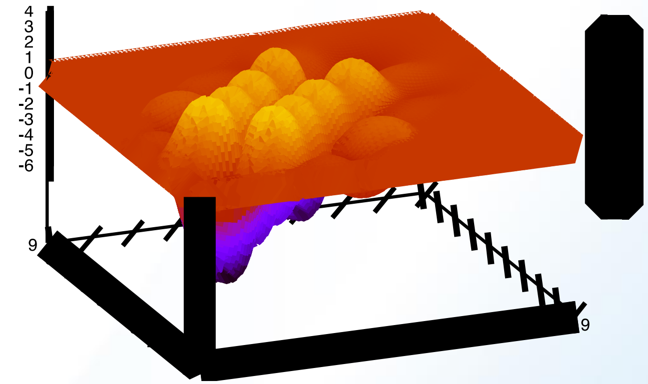
n + ^{90}Zr
E_{lab} = 40 MeV
Inelastic + transfer

Real

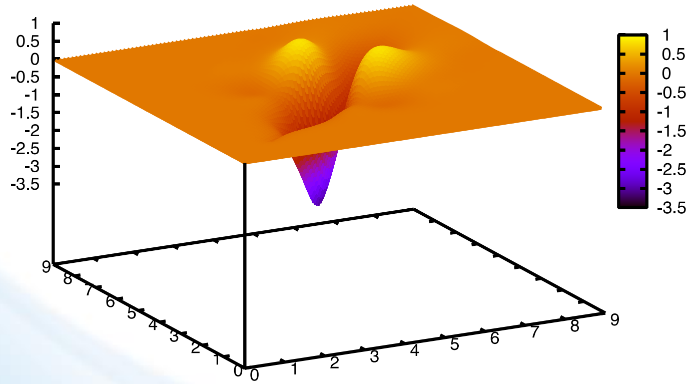
Imaginary

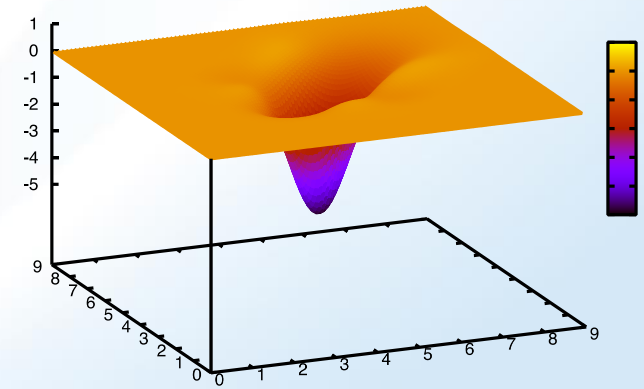
L=0



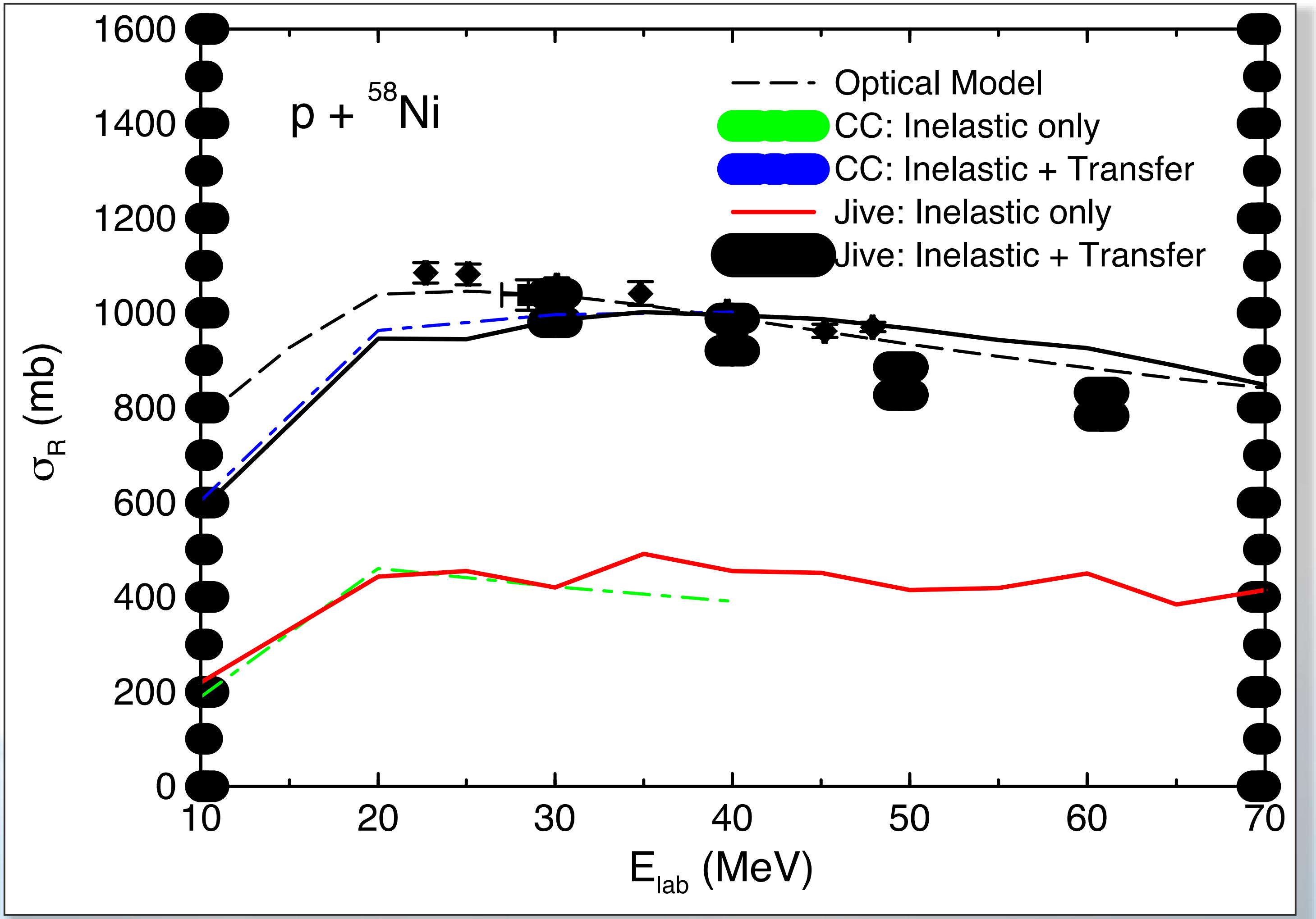


L=9
(~ grazing)





p + ^{58}Ni – Coupled Channels and Two-Step Approach



Two-step method allows to perform calculations at higher energies, coupling to higher states.

BROOKHAVEN NATIONAL LABORATORY

Conclusion

- Predictive models are crucial for progress of reaction evaluations
- Evaluations are a link between nuclear science and applications
- Collaboration with scientific community (both structure and reaction) is indispensable
- Win-win: fundamental models will improve evaluations and allow for new ones; evaluations will point new ways to go that can directly impact applications

- <u>Collaboration</u>
  - Incorporate latest theoretical models
  - Benchmark our evaluations against most recent data

References

- www.nndc.bnl.gov
- EMPIRE: Nuclear Data Sheets 108 (2007) 2655-2715
- ENDF/B library: https://ndclx4.bnl.gov/gf/project/endf/
- Soft-rotator model:
  - Physical Review C 94, 064605 (2016)
  - Physical Review C 87, 054611 (2013)
  - Nuclear Data Sheets 118 (2014) 191-194
- Rare-earths:
  - Physical Review C 91, 024618 (2015)
  - AIP Conf. Proc. 1625, 45 (2014)
  - EPJ Web of Conf. 69, 00007 (2014)
  - Nuclear Data Sheets 118 (2014) 266-269
- Nucleon-nucleus microscopic OP:
  - Physical review letters 105 (2010), 202502
  - Physical Review C 84 (2011), 064609
  - Journal of Physics: Conference Series 312 (2011), 082033
  - Computer Physics Communications 184 (2013), 2235-2250