Scientific Report

Federal Agency: NNSA/SSAA
Federal Grant: Grant DE- NA0002847
Project Title: “Theoretical Description of the Fission Process”
Principal Investigator: Witold Nazarewicz (witek@frib.msu.edu, 517-908-7326)
Submission date: June 13, 2017
DUNS Number: 193247145
Recipient Organization: Michigan State University, 426 Auditorium Rd., East Lansing MI 48824
Project period: 9/1/2016-8/31/2017
Reporting period end date: 8/31/2017

1. Accomplishments

The main goals of the project, can be summarized as follows:

i. Development of effective energy functionals that are appropriate for the description of heavy nuclei. Our goal is to improve the existing energy density (Skyrme) functionals to develop a force that will be used in calculations of fission dynamics. To this end, we use specialty Hartree-Fock (HF) and Hartree-Fock-Bogoliubov (HFB) codes.
ii. Systematic self-consistent calculations of binding energies and fission barriers of actinide, pre-actinide, and trans-actinide nuclei using modern density functionals. This is followed by calculations of spontaneous fission lifetimes and mass and charge splits using dynamic adiabatic approaches.
iii. Investigate novel microscopic (non-adiabatic) methods to study the fission process. In particular, we are going to assess whether the imaginary time method and the generator coordinate method can be used in practical self-consistent calculations.
iv. Develop codes and technology that can be freely used by NNSA researchers and, generally, by the low-energy nuclear physics community.
v. Train junior scientists and students to apply nuclear many-body techniques to describe low-energy nuclear phenomena.

We are pleased to report substantial progress in the all areas of the program. One measure of this progress is publications and invited material. During the reported period, our research resulted in 4 publications (Section 2.A). We presented our research in 13 invited and contributed talks at international meetings, colloquia, and seminars (Section 2.B). The results obtained under this project have been crucial for identifying microscopic description of fission as the forefront scientific problem in the era of extreme computing.

Our group has been very active, in terms of presentations, publications, and organizational involvement, in publicizing the research covered by this grant. Specifically:

- We presented the status of microscopic fission theory at several meetings, including SSAA Annual Workshop and several conferences in the U.S., Europe, Asia, and Australia (see below).
- We established a fission project website, https://people.nscl.msu.edu/~witek/fission/fission.html, that popularizes our research.
- Chunli Zhang received Sherwood K Haynes Award from Physics Department, MSU, for her Ph.D. work https://groups.nscl.msu.edu/userinfo/greensheets/2017/The%20Greensheet5%205%202017.pdf
- Nazarewicz served as a co-lead of a section on Nuclear Structure and Reactions of *Nuclear Physics, DOE Exascale Requirements Review report.* June 15-17, 2016. The full report can be found at http://exascaleage.org
- Our SSAA project has been highlighted in NSCL's GreenSheet: https://groups.nscl.msu.edu/userinfo/greensheets/2017/The%20Greensheet3%2031%202017.pdf
- Nazarewicz has been awarded the G.N. Flerov Prize from the Joint Institute for Nuclear Research for outstanding research in nuclear physics. He was cited for his *theoretical studies of the atomic and nuclear properties of the heaviest elements,* https://www.pa.msu.edu/node/6054

2. Products

A. Completed projects - Publications

1. *"Nucleon localization and fragment formation in nuclear fission",* C.L. Zhang, B. Schuetrumpf, and W. Nazarewicz, Phys. Rev. C 94, 064323 (2016). An electron localization measure was originally introduced to characterize chemical bond structures in molecules. Recently, a nucleon localization based on Hartree-Fock densities has been introduced to investigate α-cluster structures in light nuclei. Compared to the local nucleonic densities, the nucleon localization function has been shown to be an excellent indicator of shell effects and cluster correlations. In this work, using the spatial nucleon localization measure, we investigated the emergence of fragments in fissioning heavy nuclei using the self-consistent energy density functional method with a quantified energy density functional optimized for fission studies. We studied the particle densities and spatial nucleon localization distributions along the fission pathways of ^{264}Fm, ^{232}Th, and ^{240}Pu. We demonstrated that the fission fragments were formed fairly early in the evolution, well before scission. To illustrate the usefulness of the localization measure, we showed how the hyperdeformed state of ^{232}Th could be understood in terms of a quasimolecular state made of ^{132}Sn and ^{100}Zr fragments. Compared to nucleonic distributions, the nucleon localization function more effectively quantifies nucleonic clustering: its characteristic oscillating pattern, traced back to shell effects, is a clear fingerprint of cluster/fragment configurations. This is of particular interest for studies of fragment formation and fragment identification in fissioning nuclei.
2. "Clustering and pasta phases in nuclear density functional theory," B. Schuetrumpf, C.L. Zhang, and W. Nazarewicz, IJMPE special-topics issue on Nuclear Particle Correlations and Cluster Physics, p. 135 (2017); arXiv:1607.01372. Nuclear density functional theory is the tool of choice in describing properties of complex nuclei and intricate phases of bulk nucleonic matter. It is a microscopic approach based on an energy density functional representing the nuclear interaction. An attractive feature of nuclear DFT is that it can be applied to both finite nuclei and pasta phases appearing in the inner crust of neutron stars. While nuclear pasta clusters in a neutron star can be easily characterized through their density distributions, the level of clustering of nucleons in a nucleus can often be difficult to assess. To this end, we use the concept of nucleon localization. We demonstrate that the localization measure provides us with fingerprints of clusters in light and heavy nuclei, including fissioning systems. Furthermore we investigate the rod-like pasta phase using twist-averaged boundary conditions, which enable calculations in finite volumes accessible by state of the art DFT solvers.
3. *"Charge Radii of Neutron-Deficient ^{52,53}Fe Produced by Projectile Fragmentation",* K. Minamisono, D. M. Rossi, R. Beerwerth, S. Fritzsche, D. Garand, A. Klose, Y. Liu, B. Maass, P. F. Mantica, A. J. Miller, P. Muller, W. Nazarewicz, W. Nortershauser, E. Olsen, M. R. Pearson, P.-G. Reinhard, E. E. Saperstein, C. Sumithrarachchi, and S. V. Tolokonnikov, Phys. Rev. Lett. 117, 252501 (2016). To interpret charge radii in ^{52,53}Fe measured with bunched-beam collinear laser spectroscopy, we employed nuclear density functional theory with Fayans and Skyrme energy density functionals. We demonstrated that the trend of charge radii along the Fe isotopic chain results from an interplay between single-particle shell structure, pairing, and polarization effects. This work employed results of our systematic DFT calculations stored in the massexplorer database.

4. *"Recoil-alpha-fission and recoil-alpha-alpha-fission events observed in the reaction ^{48}Ca + ^{243}Am*, U. Forsberg, D. Rudolph, L.-L. Andersson, A. Di Nitto, Ch.E. Düllmann, J.M. Gates, P. Golubev, K.E. Gregorich, C.J. Gross, R.-D. Herzberg, F.P. Hessberger, J. Khuyagbaatar, J.V. Kratz, K. Rykaczewski, L.G. Sarmiento, M. Schädel, A. Yakushev, S. Åberg, D. Ackermann, M. Block, H. Brand, B.G. Carlsson, D. Cox, X. Derkx, J. Dobaczewski, K. Eberhardt, J. Even, C. Fahlander, J. Gerl, E. Jäger, B. Kindler, J. Krier, I. Kojouharov, N. Kurz, B. Lommel, A. Mistry, C. Mokry, W. Nazarewicz, H. Nitsche, J.P. Omtvedt, P. Papadakis, I. Ragnarsson, J. Runke, H. Schaffner, B. Schausten, Y. Shi, P. Thörle-Pospiech, T. Torres, T. Traut, N. Trautmann, A. Türler, A. Ward, D.E. Ward, and N. Wiehl, Nucl. Phys. A 953, 117 (2016). A recent high-resolution α, X-ray, and γ-ray coincidence-spectroscopy experiment at GSI offered the first glimpse of excitation schemes of isotopes along α-decay chains of Z=115. To understand these observations and to make predictions about shell structure of superheavy nuclei below ^{288}115, we employed nuclear DFT. We find that the presence and nature of low-energy E1 transitions in well-deformed nuclei around Z=110, N=168 strongly depends on the strength of the spin-orbit coupling; hence, it provides an excellent constraint on theoretical models of superheavy nuclei.

B. Presentations

1. "Prospects for breakthroughs in understanding nuclei," W. Nazarewicz, 26th International Nuclear Physics Conference, Adelaide, Australia (plenary talk), Sep. 11-16, 2016
2. "Microscopic Description of the Fission Process," W. Nazarewicz, HIAS 2016, ANU, Canberra, Australia, Sep. 18-20, 2016
3. "Survey of Reflection-Asymmetric Nuclear Deformations," Erik Olsen, 2016 DNP Fall Meeting Vancouver, BC, Canada, Oct. 13-16, 2016
4. "Nucleon localization within nuclear density functional theory," Chunli Zhang, 2016 DNP Fall Meeting, Vancouver, BC, Canada, Oct. 13–16, 2016,
5. Prospects for Breakthroughs in (Low-Energy) Nuclear Theory," W. Nazarewicz, Sixth International Conference on Fission and Properties of Neutron-Rich Nuclei Sanibel Island, Florida, November 6-12, 2016
6. "Prospects for Breakthroughs in Low-Energy Nuclear Theory," W. Nazarewicz, First Tsukuba-CCS-RIKEN joint workshop on microscopic theories of nuclear structure and dynamics, RIKEN Nishina Center, Japan, Dec. 12, 2016
7. "Large scale static and time-dependent Hartree-Fock calculations with twist-averaged boundary conditions," B. Schutrumpf, First Tsukuba-CCS-RIKEN joint workshop on microscopic theories of nuclear structure and dynamics, Tsukuba, Japan, Dec. 14, 2016
8. "The nucleon localization function in (time-dependent) DFT," B. Schutrumpf, FUSION17, Hobart, Tasmania, Australia, Feb. 23, 2017
9. "At the End of the Nuclear Chart," W. Nazarewicz, International Festive Colloquium Dedicated to the naming of the New Elements with Atomic Numbers 115, 117 and 118, RAS, Moscow, Russia, March 2, 2017
10. "Superheavy Element Research: Perspectives," W. Nazarewicz, JINR, FLNR, Dubna, Russia, March 3, 2017
11. "Microscopic Description of Fission Process," W. Nazarewicz, Stewardship Science Academic Programs (SSAP) Symposium, Naperville, IL, April 12-13, 2017
12. "Time-dependent description nuclear collisions and infinite nucleonic systems," B.

Schutrumpf, ARIS 2017, Keystone, CO, USA, May 31, 2017.
13. "Scalable nuclear density functional theory based on the code Sky3D," B. Schutrumpf, NUCLEI Meeting, Santa Fe, NM, USA, June 7, 2017.

3. Participants

Research was carried out by the principal investigator, two research professors, two postdocs, two graduate students, and a number of collaborators. A list of personnel involved in the research covered by this grant includes:

- Z. Matheson (MSU, graduate student)
- W. Nazarewicz (MSU, Principal Investigator)
- E. Olsen (MSU, postdoc)
- J. Sadhukhan (Kolkata; visiting Research Professor)
- B. Schuetrumpf (MSU, Postdoc)
- C. Zhang (MSU, graduate student; Ph.D. November 2016)

Training of next-generation nuclear theorists is an important part of our undertaking. Two graduate students were involved in our fission research: **Chunli Zhang** and **Zach Matheson.** Chunli was working on nucleon localization applications to nuclear fission, and received her Ph.D. in December 2016. Zach is involved in the analysis of fission yields around ^{176}Pt, in collaboration with experimental groups from ISOLDE and JAEA. He received the Office of Science Graduate Student Research (SCGSR) award to conduct a program for spontaneous fission calculations at LLNL, in collaboration with Dr. Nicolas Schunck.

Dr. Bastian Schuetrumpf successfully incorporated twisted angle boundary conditions into our DFT codes used for fission, including the fast-Fourier transform code. Dr. Erik Olsen is responsible for our DFT calculations and for the massexplorer database. Dr. Jhilam Sadhukhan was working with us as a postdoc and, recently, as research professor; he came from Variable Energy Cyclotron Centre, Kolkata, India. We collaborate with Dr. Nicolas Schunck (LLNL) and Dr. Patrick Talou (LANL) on microscopic theory of fission.

4. Impact

Advanced theoretical methods and high-performance computers may finally unlock the secrets of nuclear fission, a fundamental nuclear decay that is of great relevance to society. Under this project, we study the phenomenon of spontaneous fission using the symmetry-unrestricted nuclear density functional theory. Our results show that many observed properties of fissioning nuclei can be explained in terms of pathways in multidimensional collective space corresponding to different geometries of fission products. From the calculated collective potential and collective mass, we estimate spontaneous fission half-lives by minimizing the collective action integral. Our calculations demonstrate that fission barriers of excited nuclei vary rapidly with particle number, pointing to the importance of shell effects even at large excitation energies. Not only does this reveal clues about the conditions for creating new elements, it also provides a wider context for understanding other types of fission.

Understanding of the fission process is crucial for many areas of science and technology. Fission governs existence of many transuranium elements, including the predicted long-lived superheavy species. In nuclear astrophysics, fission influences the formation of heavy elements on the final stages of the r-process in a very high neutron density environment. Fission applications are numerous. Improved understanding of the fission process will enable scientists to enhance the safety and reliability of the nation's nuclear stockpile and nuclear reactors. The deployment of a fleet of safe and efficient advanced reactors, which will also minimize radiotoxic waste and be proliferation-resistant, is a goal for the advanced nuclear fuel cycles program. While in the past the design, construction, and operation of reactors were supported through empirical trials, this new phase in nuclear energy production is expected to heavily rely on advanced modeling and simulation capabilities.

Much of the research carried out under this grant has applications that can impact NNSA programs in stockpile stewardship and non-proliferation. Specifically, the research described in this proposal supports the research goals of the SSAA Program in Topic Research Area Low-Energy Nuclear Science, sub-area Physics of the fission process, including division of mass and charge as a function of excitation, production of energy, and the reaction properties of prompt fission products..

The principal impact is in the delivery of fission models capable of providing nuclear data not only of a higher quality, but also with quantified uncertainties. For many NNSA applications, the required data on fission cross sections or fission products cannot be obtained via experiment, because very neutron-rich nuclei with short half-lives are required. Understanding fission and in particular properties of fission fragments is essential to successfully analyzing fission yields under a variety of conditions.

5. Changes/Problems

There are no changes from the DOE approved application.

6. Special reporting requirements

N/A

7. Budgetary Information

We estimate no unobligated balances remaining at the end of the budget period.