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Fission In R-process Elements - FY20 Q4 Quarterly Report

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Disclaimer

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NA-22 Quarterly Report

Project Title: Fission In R-process Elements

Quarter: Q4FY20

Lab/Site/Plant: LLNL

Principal Investigator: Nicolas Schunck

HQ Project Manager: Donald Hornback

Date: 09 October 2020

Programmatic Summary

Project summary

The goal of the FIRE topical collaboration in nuclear theory is to determine the astrophysical conditions of the rapid neutron capture process (r-process), which is responsible for the formation of heavy elements. This will be achieved by including in r-process simulations the most advanced models of fission (spontaneous, neutron-induced, β-delayed) that have been developed at LLNL and LANL. The collaboration is composed of LLNL (lead) and LANL for fission work, BNL for nuclear data management, and the university of Notre Dame and North Carolina State University for r-process simulations. Under DOE/NNSA agreement, both universities receive funds from DOE Office of Science, while national laboratories receive funds directly from NA221.

Administrative News

- Erika Holmbeck and Trevor Sprouse, who were partially supported by the FIRE collaboration and contributed to its activities, graduated from Notre Dame.
- Trevor Sprouse is the new FIRE postdoc at LANL.
- Because of the covid-19 pandemic, the annual meeting of the collaboration took place online on July 1st, 2020 and was attended by 15 people.

FY20 Tasks

At the time of submission of the FIRE proposal, the submission process, which was handled by DOE/NP, did not require a breakdown in tasks for each fiscal year. Only required in the proposal was a set of annual milestones (found below with programmatic progress) and a set of deliverables for the entire project.

Milestone Progress

Task	Programmatic Progress
Task # 1 Mic-mac FPY in r-process simulations	100% complete; ahead of schedule
Task # 2 Benchmark of microscopic β-delayed fission rates	80% complete; earlier pivot to focus on full mass table calculation of β-decay rates for all nuclei
Task # 3 Potential energy surfaces with other functionals	15% complete; focus on major actinides, earlier pivot to focus on macroscopic-microscopic rather than DFT
Task # 4 β-delayed neutron emission in DFT coupled to HF	0% complete; on hold due to lack of manpower in microscopic theory
Task # 5 Neutron multiplicities	100% complete; on schedule

FY20 Deliverables

As mentioned already above, the submission process for the FIRE proposal was handled by DOE/NO and did not require a breakdown in deliverables for each fiscal year. The only deliverables required were for the entire project.

Interagency Interactions/Meetings/Conferences/Other Project Related Travel

- Ramona Vogt gave a presentation of LLNL activities at the 1st Research Coordination Meeting of the IAEA research project on fission yields of actinides

Notable Technical Highlights

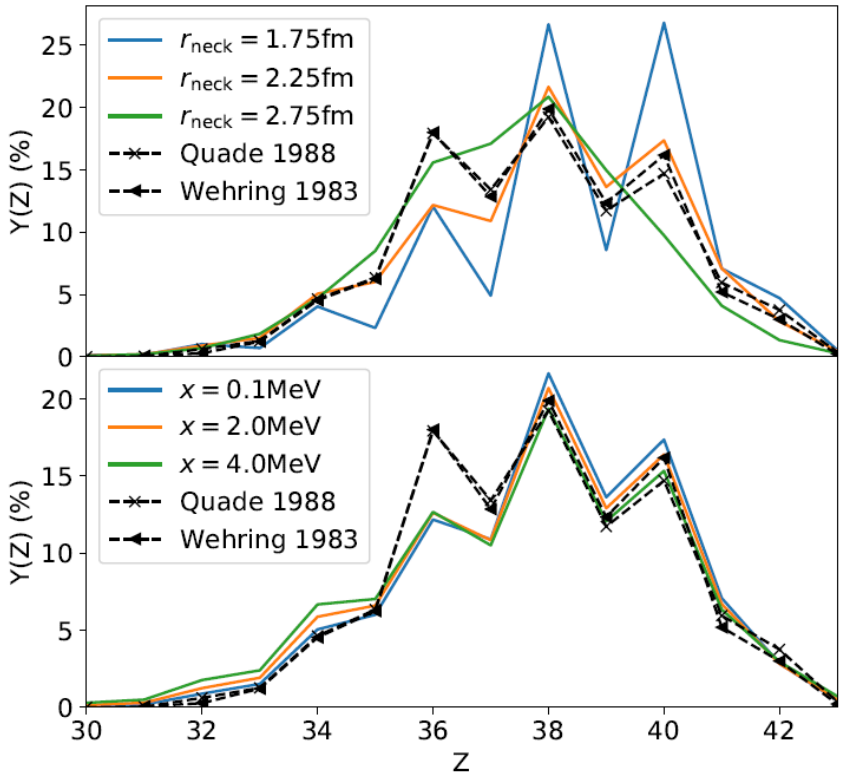

Figure 1 – Independent charge yields for ^{235}U(n,f). Top panel: yields are calculated for different sizes of the neck between the prefragments and compared with evaluations for thermal neutrons. Bottom panel: the yields are computed for different energies of the incident neutrons, thermal, 2 and 4 MeV.

Most of the fission calculations performed in the FIRE collaborations are based on the well-established macroscopic-microscopic approach to nuclear structure. In a recent work, M. Verriere and M. Mumpower, from LANL made several key enhancements to this approach that considerably increase the fidelity of theoretical predictions. They improved upon the microscopic sector of nuclear potential energy surfaces by proposing a new method to solve the Lipkin-Nogami equations' (which are used to estimate the effect of particle number projection on the pairing energy) and by eliminating spurious continuum contributions in the calculation of the shell energy with the Strutinsky procedure. They also introduced a novel deterministic method for calculating fission dynamics under the assumption of strongly damped collective motion. Their technique utilizes the memoryless property of Markov Chains to produce fission yields that do not rely on the statistical accumulation of scission events. They showed that not only is this new

technique equivalent to the Metropolis random-walk pioneered over the past decade by Randrup and colleagues, it further improves upon it, as it removes the need for altering the nuclear landscape via a biased potential. Finally, they also implemented particle number projection in the fission fragments. The charge and mass of fission fragments are thus calculated directly from the quantum mechanical A-body states of the potential energy surface rather than the collective mass asymmetry variable of the Finite-Range Liquid-Drop Model (FRLDM) used in past work. These new developments were validated by predicting for the first time the odd-even staggering and the charge polarization for the neutron-induced fission of ^{233}U and ^{235}U. Figure 1 shows the charge distribution of ^{235}U(n,f) for different neutron energies and showcases the ability of particle number projection to reproduce the odd-even staggering of this distribution.

Outlook

- LLNL nuclear data computer suite is based on slightly different physics models than the LANL codes: it relies on density functional theory (code: DFTNESS) and the time-dependent generator coordinate method (code: FELIX) for fission fragment distributions, a statistical Weisskopf-Ewing framework for particle evaporation (code: FREYA). The implementation of a new capability in FELIX to compute fission fragment distributions based not only on mean values of observables, but also distributions will allow us to cross-validate some of the FIRE results in actinide nuclei.
- The improvements to the macroscopic-microscopic framework will be applied to generating an updated table of fission fragment charge and mass distributions. Thanks to the previous work by the collaboration, such a table can now easily be plugged into simulations with either the LANL pipeline or FREYA, and subsequently be used in r process simulations themselves.

Issues/Risks

Use this section to highlight any issues (current or anticipated) with the project that HQ should be aware of.

Lab Program Manager Comments (optional)

Opportunity for lab PM commentary if needed.

Acknowledgements

This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344

Appendix

Publications (submitted)

1. Erika M. Holmbeck, Anna Frebel, G. C. McLaughlin, Rebecca Surman, Rodrigo Fernandez, Brian D. Metzger, Matthew R. Mumpower, Trevor M. Sprouse, "*Reconstructing Masses of Merging Neutron Stars from Stellar R-Process Abundance Signatures*", Submittd to ApJ [arXiv:2010.01621]
2. Xilu Wang, Nicole Vassh, Trevor Sprouse, Matthew Mumpower, Ramona Vogt, Jorgen Randrup, Rebecca Surman, "*MeV Gamma Rays from Fission: A Distinct Signature of Actinide Production in Neutron Star Mergers*", In press in ApJL [arXiv:2008.03335]

3. Erika M. Holmbeck, Rebecca Surman, Anna Frebel, G. C. McLaughlin, Matthew R. Mumpower, Trevor M. Sprouse, Toshihiko Kawano, Nicole Vassh, Timothy C. Beers, "*Characterizing r-Process Sites through Actinide Production*", Submitted to ApJ (2020) [arXiv:2001.08792]
4. B. Côté, M. Eichler, A. Yagüe, N. Vassh, M.R. Mumpower, B. Világos, B. Soós, A. Arcones, T.M. Sprouse, R. Surman, M. Pignatari, B. Wehmeyer, T. Rauscher, and M. Lugaro, "*Constraining the Rapid Neutron-Capture Process with Meteoritic I-129 and Cm-247*", Submitted to Science (2020) [arXiv:2006.04833]
5. N. Vassh, G.C. McLaughlin, M.R. Mumpower, and R. Surman, "*Markov Chain Monte Carlo Predictions of Neutron-rich Lanthanide Properties as a Probe of r-process Dynamics*", Submitted to ApJ (2020) [arXiv:2006.04322]
6. R. Vogt, J. Randrup, N. Vassh, T. Sprouse and R. Surman, "Employing FREYA for fission product yield evaluations", Submitted to EPJ Web of Conferences (2019)
7. Nicole Vassh, Matthew Mumpower, Trevor Sprouse, Rebecca Surman and Ramona Vogt, "Probing the fission properties of neutron-rich actinides with the astrophysical r process", Submitted to EPJ Web of Conferences (2020)

Publications (cumulative list)

1. E. M. Ney, J. Engel, T. Li (李通), and N. Schunck , "*Global description of β-decay with the axially deformed Skyrme finite-amplitude method: Extension to odd-mass and odd-odd nuclei*", Phys. Rev. C **102**, 034326 (2020)
2. M. R. Mumpower, P. Jaffke, M. Verriere, J. Randrup, "*Primary fission fragment mass yields across the chart of nuclides*", Phys. Rev. C **101**, 054607 (2020)
3. X. Wang, B.D. Fields, M.R. Mumpower, T.M. Sprouse, R. Surman, and N. Vassh, "*Sandblasting the r-process: Spallation of Ejecta from Neutron Star Mergers",* ApJ **893,** 92, (2020)
4. M. Verriere and D. Regnier, "*The Time-Dependent Generator Coordinate Method in Nuclear Physics",* Front. Phys. **8**, 233 (2020)
5. T. M. Sprouse, R. Navarro Perez, R. Surman, M. R. Mumpower, G. C. McLaughlin, N. Schunck, "*Propagation of Statistical Uncertainties of Skyrme Mass Models to Simulations of r-Process Nucleosynthesis*", Phys. Rev. C **101**, 055803 (2020)
6. N. Vassh, M.R. Mumpower, G.C. McLaughlin , T.M. Sprouse, and R. Surman, "*Coproduction of Light and Heavy r-process Elements via Fission Deposition",* ApJ **896,** 28, (2020)
7. Marc Verriere, Nicolas Schunck, Toshihiko Kawano, "*Number of Particles in Fission Fragments*", Phys. Rev. C **100**, 024612 (2019)
8. Erika M. Holmbeck, Anna Frebel, G. C. McLaughlin, Matthew R. Mumpower, Trevor M. Sprouse and Rebecca Surman, *Actinide-rich and Actinide-poor r-process-enhanced Metal-poor Stars Do Not Require Separate r-process Progenitors*, ApJ **881**, 5 (2019)
9. Nicole Vassh, Ramona Vogt, Rebecca Surman, Jorgen Randrup, Trevor Sprouse, Matthew Mumpower, Patrick Jaffke, David Shaw, Erika Holmbeck, Yonglin Zhu, Gail McLaughlin, "*Using excitation-energy dependent fission yields to identify key fissioning nuclei in r-process nucleosynthesis*", J. Phys. G: Nucl. Part. Phys. **46**, 065202 (2019)
10. Erika M. Holmbeck, Trevor M. Sprouse, Matthew R. Mumpower, Nicole Vassh, Rebecca Surman, Timothy C. Beers and Toshihiko Kawano, "*Actinide Production in the Neutron-rich Ejecta of a Neutron Star Merger*", ApJ **870**, 23 (2019)
11. A.A. Sonzogni, M. Nino, E.A. McCutchan, "*Revealing fine structure in the antineutrino spectra from a nuclear reactor*", Phys. Rev. C **98**, 014323 (2018)

12. Y. Zhu, R.T. Wollaeger, N. Vassh, R. Surman, T.M. Sprouse, M.R. Mumpower, P. Moeller, G.C. McLaughlin, O. Korobkin, T. Kawano, P.J. Jaffke, E.M. Holmbeck, C.L. Fryer, W.P. Even, A.J. Couture, J.Barnes, "*Californium-254 and Kilonova Light Curves*" ApJL **23**, 863 (2018)
13. M. R. Mumpower, T. Kawano, T. M. Sprouse, N. Vassh, E. M. Holmbeck, R. Surman, and P. Möller, "*β-delayed Fission in r-process Nucleosynthesis*", ApJ **869**, 14 (2018)
14. Shin Okumura and Toshihiko Kawano and Patrick Jaffke and Patrick Talou and Satoshi Chiba, "*235U(n,f) Independent Fission Product Yield and Isomeric Ratio Calculated with the Statistical Hauser-Feshbach Theory*", J Nucl. Sci. Technol. **55**, 1009 (2018)
15. Benoit Côté, Chris L. Fryer, Krzysztof Belczynski, Oleg Korobkin, Martyna Chruślińska, Nicole Vassh, Matthew R. Mumpower, Jonas Lippuner, Trevor M. Sprouse, Rebecca Surman, and Ryan Wollaeger, "*The Origin of r-process Elements in the Milky Way*", ApJ **855**, 99 (2018)
16. R. Orford, N. Vassh, J. A. Clark, G. C. McLaughlin, M. R. Mumpower, G. Savard, R. Surman, A. Aprahamian, F. Buchinger, M. T. Burkey, D. A. Gorelov, T. Y. Hirsh, J. W. Klimes, G. E. Morgan, A. Nystrom, and K. S. Sharma, "*Precision Mass Measurements of Neutron-Rich Neodymium and Samarium Isotopes and Their Role in Understanding Rare-Earth Peak Formation*" Phys. Rev. Lett. **120**, 262702 (2018)
17. A.C. Hayes, Gerard Jungman, E.A. McCutchan, A.A. Sonzogni, G.T. Garvey, X.B. Wang, "*Analysis of the Daya Bay Reactor Antineutrino Flux Changes with Fuel Burnup*" Phys. Rev. Lett. **120**, 022503 (2018)
18. X. B. Wang and A. C. Hayes, *"Weak magnetism correction to allowed β-decay for reactor antineutrino spectra*", Phys. Rev. C **95**, 064313 (2017)
19. M. R. Mumpower, T. Kawano, J. L. Ullmann, M. Krtička, T. M. Sprouse, *"Estimation of M1 scissors mode strength for deformed nuclei in the medium to heavy mass region by statistical Hauser-Feshbach model calculations*", Phys. Rev. C **96**, 024612 (2017)
20. A.A. Sonzogni, E.A. McCutchan, T.D. Johnson, P. Dimitriou, "*Effects of Fission Yield Data in the Calculation of Antineutrino Spectra for 235U (n, fission) at Thermal and Fast Neutron Energies*", Phys. Rev. Lett. **116**, 132502 (2016)
21. M. Mumpower, T. Kawano, P. Möller, "*Neutron-gamma competition for β-delayed neutron emission*", Phys. Rev. C **94**, 064317 (2016)

Talks

1. N. Vassh, "*Exposing the astrophysical conditions of r-process events through observable signatures of lanthanide and actinide production"*, Network for Neutrinos, Nuclear Astrophysics, and Symmetries (N3AS) Collaboration Online Seminar, Jun. 2, 2020
2. N. Vassh, "*Impact of examining neutron-rich lanthanides and pushing the bounds into neutron-rich actinides on r-process nucleosynthesis calculations"*, FRIB First Experiments: Proposal Preparation Workshop, JINA-CEE organized event, May 5, 2020
3. N. Vassh, "*The impact of fissioning nuclei on r-process nucleosynthesis observables"*, APS Virtual April Meeting 2020, L04 Invited Session: Sensitive Reaction Studies for Nuclear Astrophysics, Apr. 19, 2020
4. N. Schunck, "*The FIRE (Fission In R-process Elements) Topical Collaboration*", DOE/NSF Nuclear Science Advisory Committee Meeting, Washington DC, Mar. 2, 2020
5. N. Vassh, "*Examining lanthanide production in merger accretion disk winds: nuclear masses and the rare-earth peak"*, Argonne National Laboratory, Physics Division Seminar, Feb. 24, 2020

6. R. Vogt, "*Modeling fission events in the lab and the universe"*, Physics Department Colloquium, San Diego State University, Jan. 4, 2020
7. N. Vassh, "*r-process nucleosynthesis studies meet the next generation of observation and experiment*", Michigan State University, FRIB Theory Seminar, Dec. 2, 2019
8. M. Mumpower, "*FRLDM fission yields for r-process nucleosynthesis*", Workshop on Nuclear Astrophysics, Beihang University, China, Nov. 28, 2019
9. Rebecca Surman, "*r process: synthesizing observations, simulation, and nuclear physics"*, RPA workshop, MIT, Nov. 21, 2019
10. Rebecca Surman, "*Nuclear structure of exotic nuclei and astrophysical nucleosynthesis*", Gogny 2019, LLNL, Nov. 12, 2019
11. N. Vassh, "*Potential signatures of fission in the r-process*", Washington University, Nuclear Theory Seminar, Nov. 8, 2019
12. M. Mumpower, "*Fission across the chart of nuclides and implications for the r-process*", Workshop on Nuclear Fission Dynamics, Kyoto University, Oct. 28, 2019
13. Rebecca Surman, "*Neutron star mergers and the origins of the heaviest elements"*, colloquium, Penn State University, Oct. 24, 2019
14. Rebecca Surman, "*Forging the heaviest elements"*, colloquium, Illinois State University, Oct. 22, 2019
15. N. Vassh, "*Macroscopic-Microscopic fission yields for nucleosynthesis"*, APS DNP 2019 Fall Meeting, Oct. 16, 2019
16. N. Vassh*, "Examining lanthanide production in merger accretion disk winds: nuclear masses and the rare-earth peak"*, APS DNP 2019 Fall Meeting, Oct. 16, 2019
17. R. Vogt, "*Employing FREYA as a tool for fission product yield evaluations*", Fission Product Yields (FPY) Workshop 2019, Sept. 30 - Oct. 3, 2019
18. T. Sprouse, "*Following fission products in explosive astrophysical environments*", Fission Product Yields (FPY) Workshop 2019, Sept. 30 - Oct. 3, 2019
19. R. Surman, "*Fission and the origins of the heaviest element*", Fission Product Yields (FPY) Workshop 2019, Sept. 30 - Oct. 3, 2019
20. N. Vassh, "*Fission and lanthanide production in r-process nucleosynthesis"*, Fission Product Yields (FPY) Workshop 2019, Sept. 30 - Oct. 3, 2019
21. R. Vogt, *Fission Modeling for Correlated Observables*, Notre Dame nuclear physics seminar, 09/16/2019
22. N. Vassh*, "r-process nucleosynthesis in compact object mergers"*, Microphysics In Computational Relativistic Astrophysics (MICRA) Workshop, August 12-16, 2019
23. G. McLaughlin, "*Nuclear Physics of Neutron Star Mergers*", FRIB Low-Energy Community Meeting, August 8, 2019
24. R. Vogt, *Detailed Modeling of Fission and Some Implications for the Astrophysical r process*, Frankfurt Institute for Advanced Study colloquium, July 3, 2019
25. N. Vassh, "*Fission and lanthanide production in r-process nucleosynthesis"*, Institute for Nuclear Theory, S@INT Seminar, June 6, 2019
26. N. Vassh, *"Identifying the neutron-rich nuclei that most influence heavy element abundances: fission and the rare-earth peak*", JINA Frontiers Conference, May 22-24, 2019
27. N. Vassh, "*Fission and lanthanide production in r-process nucleosynthesis"*, SouthEast Laboratory Astrophysics Community (SELAC) Conference, May 13-16, 2019

28. N. Vassh*, "Fission and lanthanide production in r-process nucleosynthesis"*, R-process Sources in the Universe JINA-CEE conference, March 27-30, 2019
29. N. Vassh, *"Fission and lanthanide production in r-process nucleosynthesis"*, University of Maryland, Nuclear Physics Seminar, March 6, 2019
30. N. Vassh, *"Fission and lanthanide production in r-process nucleosynthesis"*, University of California - San Diego, Astrophysics Seminar, Feb. 6, 2019
31. G. McLaughlin, "*Neutrino and Nuclear Physics of the r-process*", Colloquium, APC Laboratory, Paris, France December 14, 2018
32. R. Surman, "*GW170817 and the origins of the heaviest elements*", Colloquium, Department of Physics, Rutgers University, November 7, 2018
33. N. Vassh, "*The formation of the rare-earth peak in neutron star mergers*", 5th Joint Meeting of the APS Division of Nuclear Physics and the Physical Society of Japan, October 23-27, 2018
34. N. Vassh, "*Examining the origin of the r-process rare earth peak with Markov Chain Monte Carlo*", Uncertainty Quantification at the Extremes (ISNET-6), TU Darmstadt, October 8-12, 2018
35. G. McLaughlin, "*Neutrino and Nuclear Physics of the r-process*", Colloquium, College of William and Mary, Williamsburg, VA, October 2018
36. R. Surman, "*The microphysics of the GW170817 kilonova*", Colloquium, Department of Physics, University of Massachusetts Lowell, September 26, 2018
37. R. Surman, "*Nuclear physics and the r process*", To 2020 and Beyond: Radionuclide Astronomy, Los Alamos National Laboratory, August 20-22, 2018
38. M. Mumpower, "*Recent progress on Los Alamos nuclear structure, reaction and fission models*", Nuclear Structure 2018, MSU, August 2018
39. N. Schunck, "*Theories of Nuclear Fission*", FRIB and the GW170817 kilonova, MSU, July 16-27, 2018
40. M. Mumpower, "*Fission in the r-process*", Ariel Science Week, Triumf, Vancouver, July, 2018
41. G. McLaughlin, "*Neutron Star Mergers*", Workshop on Quantum Kinetic Equations, Santa Fe, NM, July 1-7, 2018
42. G. McLaughlin, "*Theoretical aspects of nuclear astrophysics*", National Nuclear Physics Summer School, June 17-30, 2018P. Jaffke, "*Correlations between the fission fragment yields and the prompt fission gamma-ray spectrum*", 15th International Conference on Nuclear Reaction Mechanisms, Varenna, June 11-15, 2018
43. N. Vassh, "*Studying lanthanide production in r-process nucleosynthesis*", Conference on the Intersections of Particle and Nuclear Physics (CIPANP) June 2018
44. N. Vassh, "*Reverse engineering properties of neutron-rich lanthanides by examining the r-process rare earth abundance peak*", INT-JINA Symposium: "First multi-messenger observations of a neutron star merger and its implications for nuclear physics" March 2018
45. N. Vassh, "*Fission and the Formation of the r-process Rare-Earth Abundance Peak in Neutron Star Mergers*", MSU FRIB Theory Seminar March 1, 2018 and UW-Madison NPAC Seminar May 2018
46. R. Surman, *"Understanding the r process through nuclear data*", 232nd Meeting of the American Astronomical Society, Denver, CO, June 3-7, 2018
47. R. Surman, "*The astrophysical origins of the heaviest elements*", Colloquia at Michigan State April 5, 2018 and LANL March 2018
48. N. Vassh, "Fission and the formation of the r-process rare-earth abundance peak in neutron star mergers", LBNL Nuclear Science Division Seminar, February 2018

49. N. Vassh, "*The r-process in neutron star mergers*", Neutrinos, Nuclear Astrophysics, and Symmetries (N3AS) Collaboration Meeting, UC San Diego, CA, January 2018
50. R. Surman, "*r-process nucleosynthesis and radioactivity in merger ejecta*", KITP Program GW170817: The First Double Neutron Star Merger, 2017, Kavli Institute, Santa Barbara, CA, December 2017
51. N. Vashh, "*Recent results of reverse engineering nuclear masses from solar r-process abundances and the challenges faced in the presence of fissioning nuclei*", DNP Fall Meeting, Pittsburgh,
52. P. Jaffke, "*Implementing and testing theoretical fission fragment yields in a Hauser-Feshbach statistical decay framework*", Scientific Workshop on Nuclear Fission Dynamics and the Emission of Prompt Neutrons and Gama Rays, Varna, Bulgaria, June 20-22, 2017
53. R. Surman, "*Astrophysical Alchemy*", colloquium, Ball State University, Muncie, IN, April 2017
54. R. Surman, "*Nuclear masses and the site of r-process nucleosynthesis*", invited talk, Nuclear Physics in Astrophysics VIII, Catania, Sicily, June 2017
55. R. Surman, "*Nuclear physics inputs for nucleosynthesis*", review talk, INT-17-2b Electromagnetic Signatures of r-Process Nucleosynthesis in Neutron Star Binary Mergers, Institute of Nuclear Theory, Seattle, WA, July 2017
56. G. C. McLaughlin, "*Theory Initiatives*", NSAC Meeting, June 2017

Posters

1. N. Vassh, "*Examining the astrophysical site of r-process nucleosynthesis by reverse engineering nuclear properties from rare earth abundances*", ARIS 2017, Keystone CO, May 2017