



The Nuclear Process Science Initiative (NPSI) is a Pacific Northwest National Laboratory (PNNL) internally-funded effort to advance nuclear process science capabilities to meet national needs in environmental management, nonproliferation and other areas. The five-year initiative was launched in mid-2015.

***NPSI's vision** is to understand, harness, and exploit interfacial phenomena controlling the behavior of materials in nuclear processing.*

Researchers are working in three "thrust" areas:

Science Thrust 1:
Linking Interfacial Phenomena to Bulk Properties

Science Thrust 2:
Interfacial Phenomena Driving Chemical Fractionation

Science Thrust 3:
Radiation-driven Interfacial Reactivity.

November 2017

Reid's Notes

NPSI Completes Another Year...Achieves Key Advances...Moves Forward with New Initiative Leadership

By Reid Peterson, Initiative Lead

We closed out fiscal year (FY) 2017 in September, marking another 12 months of great progress for the Nuclear Process Science Initiative. During the year, our research led to knowledge that will inform future environmental management and nonproliferation-related solutions, we secured new external funding for PNNL based on NPSI advances, and our researchers published in key journals. We continue to benefit from a NPSI team that includes a diverse blend of talented senior, mid-level and early-career staff.



As we move forward in FY 2018, there's a leadership change to report. I was recently selected to succeed **Sue Clark** as initiative lead. Sue became the Chief Science and Technology Officer in PNNL's Energy and Environment Directorate (EED) in September, and now works across the directorate to ensure science and technology development and deployment remain cutting-edge and best-in-class. She also oversees the

NPSI Leadership:

Initiative Lead: Reid Peterson
Deputy Lead: Matt Douglas
Thrust 1 Lead: Reid Peterson
Thrust 2 Lead: Jon Schwantes
Thrust 3 Lead: Kevin Rosso
Project Coordinator: Barb Beller
Finance: Debbie Lucas
Communications: Tim Ledbetter

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Jaehun Chun Receives KIChE's Lee Memorial Award

One of NPSI's principal investigators, Jaehun Chun, has been honored by the Korean Institute of Chemical Engineers (KIChE), U.S. Chapter, for his exceptional leadership in chemical engineering.

Chun received the James M. Lee Memorial Award, which acknowledges the work of mid-career Korean and Korean-American scientists, on November 1 at the American Institute of Chemical Engineers (AIChE) Annual Meeting in Minneapolis. As part of the award, Chun presented a lecture at the annual meeting's KIChE Open Forum.

"It's a great honor to receive this prestigious award that pays tribute to and reflects the values of James M. Lee, a prominent leader in the chemical engineering field. The award indeed results from constructive collaboration with

EED-stewarded Laboratory Directed Research and Development initiatives, including NPSI, so we will continue to benefit from Sue's insights and advice. We are grateful for her leadership and many contributions to NPSI.

I'm well acquainted with NPSI, having played a role in the exploratory activities that led to its formation. Since NPSI's launch, I have guided the initiative's research thrust focused on linking interfacial phenomena to bulk properties. For more info on my background and experience, check out my [bio](#) on the NPSI website.

I look forward to working with a great NPSI team to advance PNNL's nuclear science capabilities. We've accomplished a lot already, and I'm confident we'll achieve even greater impact in the future.

Reid

Research Spotlight: NPSI Publication on Particle Study Method Includes Video

A new NPSI-developed technique for studying particles in liquid using high-vacuum scanning electron microscopy (SEM) serves as the basis for a great journal paper, but NPSI researchers are also showcasing their discovery in a very visual way.

When the Journal of Visualized Experiments (JoVE) accepts a paper, authors work with the peer-reviewed publication to create a video to accompany the written product. "I believe it makes it easier for other researchers to duplicate our method if they can see how we do it," says PNNL's Xiao-Ying Yu, who led submission of the NPSI paper to JoVE and the subsequent video development.



Xiao-Ying Yu

The paper, "In Situ Characterization of Boehmite Particles in Water Using Liquid SEM," outlines a

colleagues," Chun says. Chun leads the NPSI project, "Correlation of Colloidal Interactions and Macroscopic Rheology in Concentrated Electrolyte Solutions."

According to KIChE, Professor Lee played a seminal role in chemical engineering, and nearly every practitioner in this field was associated with him, directly or indirectly. His example, counsel, and advice impacted countless Korean-American scientists and engineers, encouraging them to seek excellence in teaching, research, and professional contributions to basic and interdisciplinary science and engineering.

The award recipient must be a principal investigator of Korean descent affiliated with a U.S. institution of higher education, national laboratory, industrial laboratory or non-profit research organization.



Jaehun Chun (left) received his award at the AIChE Annual Meeting. Here he's shown with Hyunmin Yi, an associate professor at Tufts University and a KIChE award committee chair.

technique developed in the NPSI project led by Jaehun Chun. The technique offers several advantages over existing methods and will help answer key questions in the microscopy and microanalysis field, such as how to characterize evolving particle size and morphology corresponding to environmental changes.

The paper was submitted to JoVE earlier this year. It went through technical peer review and editorial review for procedure clarity, and then Yu worked with the journal staff to create a video script. JoVE dispatched a videographer to PNNL this past summer to tape interviews with the research team and capture the technique on video.

"After that, we iterated edits on the video with JoVE," Yu says. She notes that developing a precise video script at the outset is an important step that helps minimize the need for later, more time-consuming edits. She adds that while the journal's paper and video approach is still somewhat novel, it isn't entirely new to her and others at PNNL. She has produced one other paper-video combination for dissemination of new techniques.

The [paper and video were published](#) in September. In addition to Yu and Chun, other authors, most of whom are featured in the video, are Juan Yao, Bruce Arey, Li Yang, Fei Zhang and Rachel Komorek.

NPSI Receives Good Marks From Annual Review

The Nuclear Process Science Initiative's Annual Review was held July 12-13 at Pacific Northwest National Laboratory. Following the two-day meeting, NPSI's Advisory Board concluded that the initiative is delivering solid, cutting-edge science and enduring capabilities for PNNL. The group also identified areas for improvement and provided ideas for strengthening NPSI going forward.

The meeting included overview presentations given by NPSI leadership, a tour of the Radiochemical Processing Laboratory, and a poster session that provided research staff an opportunity to update



Chun presents a lecture at the KIChE Open Forum.

Initiative Launches Four New Projects

Four new projects are getting under way as NPSI begins its third year.

"Dissolution of Spent Nuclear Fuel: An In-situ and Atomic Resolution TEM Study," will be led by Edgar Buck. The Thrust Area 1 project focuses on advancing PNNL's efforts in spent nuclear fuel chemistry at the sub-micrometer scale and increasing the expertise base in the corrosion of nuclear fuels.

The other three projects are in Thrust Area 3:

"Determining Radiolytic Transient Intermediates and Interfacial Species and Their Roles in Aluminum Oxyhydroxide Reactivity," is developing a suite of unique spectroscopic techniques

Advisory Committee members on NPSI projects. The review also featured presentations by PNNL leadership on advances in the Laboratory's nuclear capabilities and other programs.

Participating Advisory Committee members were **Karthik Subramanian** (chair), Washington River Protection Solutions; **Dawn Wellman** (secretary), PNNL; **Chris Aardahl**, PNNL; **Chris Cahill**, George Washington University; **Andy Felmy**, Washington State University; **David LaGraffe**, DOE National Nuclear Security Administration; **Chris Mundy**, PNNL; **Glenn Sjoden**, Air Force Technical Applications Center; and **William Ulicny**, DOE Office of Intelligence and Counterintelligence.



NPSI's Annual Review included group discussions, this one involving Dawn Wellman (foreground) and, from left, Jon Schwantes (NPSI Thrust Area 2 Lead), Chris Cahill and Karthik Subramanian.

Annual Review Poster Session Provides View into NPSI Projects

More than 20 posters were developed and shared with the NPSI Advisory Committee at the Annual Review poster session, held July 12 in EMSL, the Environmental Molecular Sciences Laboratory, a U.S. Department of Energy national scientific user

designed to investigate transient species at solid-water interfaces in real time. The project is led by Zheming Wang.

"Characterization of Radiation Induced Defects Across Scales," is led by Luke Sweet and focuses on developing a method for characterizing and quantifying defect microstructures in nuclear materials across scales from TEM-accessible (pm) up to XRD accessible (cm).

"Damage Mechanisms and Defect Formation in Irradiated Model Systems," is led by Principal Investigator Steven Spurgeon and Co-Lead Michel Sassi. The project seeks to achieve predictive insight into the key factors that drive irradiation-induced defect formation in model systems using atomic-resolution STEM imaging and density functional theory (DFT) simulations.

Howett Earns Recognition at Postdoc Event

NPSI researcher Susan Howett was named the winner of the Post Doctorate Poster Session at PNNL's 9th Annual Post Graduate Research Symposium, July 25-26.



Howett

"I was very surprised to hear I had won, and am looking forward to using

facility located at PNNL. The poster session's flavor is captured in the video and photos below.

Video:

NPSI researcher **Philip Schonewill** discusses the goals of the NPSI project, "Particle-Filter Surface Interactions and Dynamics in the Presence of Cross-Flow," which is led by Richard Daniel. [View video.](#)



From left, Advisory Committee members William Ulicny and Karthik Subramanian discuss the Rad AFM project with researcher Carolyn Pearce and Principal Investigator Greg Kimmel.



Principal Investigator Amanda Casella (at right) discusses outcomes from her project, "Interfacial Diffusion and Crud Formation at the Liquid-Liquid Interface of Solvent Extraction Processes," with, from left, NPSI's Jon Schwantes and Advisory Committee member Glenn Sjoden.

the travel prize to attend a conference next year," Howett says.

Her poster, "Interfacial Diffusion and Crud Formation at the Liquid-Liquid Interface of Solvent Extraction Processes," is based on work from the NPSI project of the same name. The poster was one of 13 in the session.

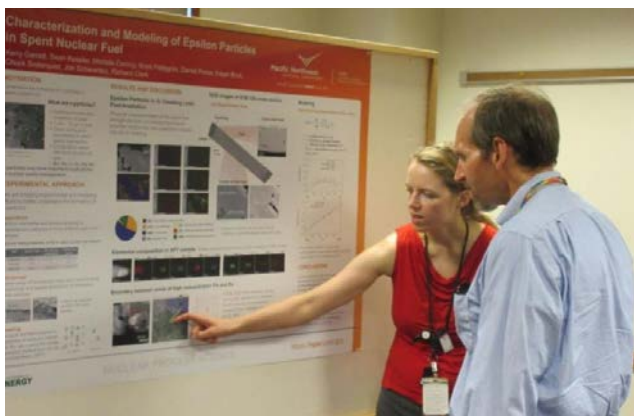
"As an early career scientist, the symposium was an excellent venue to share my early findings and have frank discussions regarding the results and data interpretation," Howett explains. "I gained valuable input, with respect to both data treatment and instrument capabilities, from meeting with various colleagues."

NPSI's Kerry Garrett also presented a poster at the event, representing work from the initiative's project, "Monitoring Diffusion of Actinide Daughters and Granddaughters in Metals for Chronometer Applications."

The symposium featured lightning talks, oral presentations and two separate poster sessions showcasing the work of PNNL's Post Bachelors, Masters and Doctorate Research Associates.

New Postdocs Support Initiative

Jacob Bair and Andrew Ritzmann joined PNNL in August as postdoctoral research assistants and are supporting the NPSI project, "Development of Phase Field



NPSI Deputy Lead Matt Douglas (foreground) learns from researcher Kerry Garrett about the progress of the project, "Modeling the Interfacial Effects, Partitioning, and Production Routes of Epsilon Particles in Uranium Oxide."

NPSI Publications and Presentations

April-November

Journal Articles:

Conroy M.A., J.A. Soltis, R.S. Wittman, F.N. Smith, S. Chatterjee, X. Zhang, E.S. Ilton and E.C. Buck. "Importance of Interlayer H Bonding Structure to the Stability of Layered Minerals." Scientific Reports (Published online). [DOI: 10.1038/s41598-017-13452-7](https://doi.org/10.1038/s41598-017-13452-7).
[See NPSI website news article.](#)

Yao J., B. Arey, R. Komorek, F. Zhang, J. Chun, and X.Y. Yu. "In Situ Characterization of Boehmite Particles in Water Using Liquid SEM." J. Vis. Exp. (127), e56058. [DOI: 10.3791/56058](https://doi.org/10.3791/56058).

Shen Z, E.S. Ilton M.P. Prange, S.N. Kerisit. "Molecular Dynamics Simulations of the Interfacial Region Between Boehmite and Gibbsite Basal Surfaces and High Ionic Strength Aqueous Solutions." Journal of Physical Chemistry C, 121(25): 13692-13700. [DOI: 10.1021/acs.jpcc.7b02463](https://doi.org/10.1021/acs.jpcc.7b02463).

Pednekar S., J. Chun and J. Morris. 2017. "Simulation of Shear Thickening in Attractive Colloidal Suspensions." Soft Matter, 13(9): 1773-1779. [DOI: 10.1039/C6SM02553F](https://doi.org/10.1039/C6SM02553F).
(Image from paper was used in journal's inside front cover).

Presentations:

Howett S.E., A.J. Casella, A.M. Lines, D.R. Bottenus, S.B. Clark, C.A. Louie, C.H. Delegard, S.A. Bryan, G.J. Lumetta, W.K. Pitts, and K.M. McCoy. 2017. "Liquid:Liquid Interfacial Reactions and Phase Transfer Kinetics during Solvent Extraction." Presented

Modeling to Predict Morphologies of Plutonium Oxalate."

Bair earned a bachelor's degree in Mechanical Engineering with a second major in French

from Washington State University in December 2012, then his Ph.D. in Materials Science and Engineering from Missouri

University of Science and

Technology in December 2016. His research has focused on

experimental and computational studies of the microstructural evolution of materials using scanning electron microscopy with Electron Backscatter Diffraction, Phase Field Modeling, and Molecular Dynamics.



Bair

Ritzmann earned his Ph.D. in Chemical Engineering from Princeton

University. He works on

modeling the

thermodynamic and kinetic behavior of actinide materials. He previously analyzed oxygen ion transport in fuel cell materials using density functional theory and developed microkinetic models of carbon dioxide reduction.



Ritzmann

by Susan E. Howett at American Chemical Society Northwest Regional Meeting, June 27, 2017, Corvallis, OR.

Heller F.D., S. Chatterjee, W.C. Isley III, S.M. Kathmann, J.A. Soltis, M.A. Conroy, E.C. Buck, Z. Wang, G.B. Hall, A.J. Casella, and G.J. Lumetta. 2017. "**Understanding Kinetics of Europium(III) Oxalate Nucleation.**" Presented by Forrest D. Heller at American Chemical Society Northwest Regional Meeting, June 25, 2017, Corvallis, OR.

Kessler S.H., D.G. Abrecht and D.E. Meier. 2017. "**Thermodynamic Modeling of Plutonium (IV) Oxalate Precipitation.**" Actinide Separations Conference, May 23, 2017, Chicago, IL.

Howett S.E., A.J. Casella, A.M. Lines, D.R. Bottenus, S.B. Clark, C.A. Louie, C.H. Delegard, G.J. Lumetta, W.K. Pitts and K.M. McCoy. 2017. "**Complexation and Phase Transfer Kinetics of Tributyl Phosphate Degradation Products at the Liquid:Liquid Interface during Solvent Extraction.**" Presented by Susan E. Howett at 253rd American Chemical Society National Meeting and Exposition, April 4, 2017, San Francisco, CA.

Kerisit S.N., M.P. Prange, Z. Shen, X. Zhang, L. Kovarik, E.S. Ilton and K.M. Rosso. 2017. "**Aluminum Oxyhydroxide-water Interfaces: Structure, Energetics, and Effects of γ -radiation.**" Presented by Sebastien N. Kerisit at 253rd American Chemical Society National Meeting and Exposition, April 4, 2017, San Francisco, CA.