BROOKHAVEN NATIONAL LABORATORY
PROPOSAL INFORMATION QUESTIONNAIRE
LABORATORY DIRECTED RESEARCH AND DEVELOPMENT PROGRAM

PRINCIPAL INVESTIGATOR	**Vanessa Sanders (MIRP/CAD)**	**PHONE**	**631-344-7230**
DEPARTMENT/DIVISION	**C-AD/NE - NPP/EBNN**	**DATE**	**6/7/2021**
OTHER INVESTIGATORS	**Alejandro Sonzogni (NSTD), Anibal Boscoboinik (CFN), Dario Stacchiola (CFN), Elizabeth McCutchan (NSTD), Chris Morse (NSTD),**		
TITLE OF PROPOSAL **TYPE A**	**TRAPPING NOBLE GASES IN SILICATE NANOCAGES FOR MEDICAL ISOTOPES, NUCLEAR ENERGY, AND NUCLEAR NONPROLIFERATION**		
PROPOSAL TERM (month/year)	From **October/2021**	Through	**September/2024**

SUMMARY OF PROPOSAL

Description of Project: Prior work at BNL showed that two-dimensional silicates made of polygonal prism nanocages could trap single atoms of noble gases at room temperature and aid in separating noble gas mixtures. The cages forming the silicates provide a perfect fit for single atoms of all noble gases larger than neon, including Ar, Kr, Xe, and Rn, which enter the cages as charged ions before getting trapped in the neutral state. The single atoms remain in the cages up to unprecedentedly high temperatures (Kr: 523 K, Xe: 723 K, and Rn: 773 K). Immobilizing noble gas atoms in a controlled way has a wide range of potential applications. These include radiological medical isotopes, safer nuclear energy production, and U.S. government nuclear nonproliferation programs. Recent unpublished data acquired at BNL has shown that potentially scalable synthesis procedures result in a material that can successfully trap these gases. We propose to produce silicate cage materials tailored for isotope production and nuclear applications and study the trapping of noble gases (including isotopes of Kr, Xe, and Rn) at relevant conditions.

Expected Results: The results will improve our understanding of the trapping of isotopes of noble gases in silicate nanocages and enable various new research areas within different directorates at BNL. This can lead to several potential uses aligned with the DOE mission and Brookhaven lab's initiatives in relation to 1. Nuclear Physics; 2. Clean Energy and Climate, and 3. Isotope Production. We intend to produce silicate cages to study the fundamental understanding of the decay chains following nuclear detonation events through analyzing trapped Kr and Xe isotopes. We further anticipated developing a trapping device from the silicate cages that will facilitate the mitigation of gaseous release from target processing and nuclear waste sites. We also expect the results from this proposal to lead to future funding from the Department of Energy (DOE), including the Early Career Award, Isotope Production and Nuclear Nonproliferation (NA-22) opportunities. We further anticipate the use of these applications allowing for funding opportunities from outside agencies such as the Department of Defense (DOD) and the National Institutes of Health (NIH).

PROPOSAL

Separations of chemicals, including gases, are energy intensive processes affecting numerous applications from catalysis to nuclear energy. Immobilizing single atoms of noble gases on a surface is fundamentally interesting as it allows their detailed study in confinement using surface science methods. Aside from the fundamental aspects, trapping noble gases at 300 K and higher temperatures can have important implications in various areas related to the use and/or control of radiological inert gases.

Recent serendipitous work at BNL showed that single Ar atoms can be trapped in sub-nanometer hexagonal prism silicate cages. [1] These cages are the building blocks of a two-dimensional (2D) material, [2,3] grown on a metallic support. The side and top views of the structure are shown in Figs. **1a** and **b**. A scanning tunneling microscopy (STM) image of the hexagonal network is shown in Fig. **1c**. Trapping of noble gas atoms was demonstrated *in situ* using ambient pressure X-ray photoelectron spectroscopy (AP-XPS) at beamline 23-ID-2 of NSLS-II. [1] Fig. **1d** depicts trapping a single noble gas atom in one of the cages. XPS spectra of Ar, Kr and Xe trapped at 300 K are shown in Fig. **1e**. The noble gases remain in the cages upon returning to ultra-high vacuum (UHV) conditions. Density functional theory (DFT) calculations predict that Rn should follow the same behavior. [4] Unpublished DFT calculations also show that noble gas atoms are stable in the cages of the free-standing structures, i.e.: without the metallic support.

Potential new areas of research cutting across three directorates at BNL have been identified in discussions involving the PI (Sanders) and other investigators (Sonzogni, Boscoboinik) in this proposal. Four of these areas relate to radiological gases and are the main focus of this proposal. These are (1) Medical Isotopes (Xe-129/127, and Rn-211 decay to the alpha emitter At-211,), (2) U.S. Government Nuclear Non-Proliferation Programs (counting of Xe-133 is used to identify instances of nuclear testing), (3) Fundamental understanding of the decay of Kr and Xe isotopes, and (4) Nuclear Energy (in nuclear power plants, the release of radioactive Kr and Xe to the atmosphere is currently hard to control due to the lack of a suitable material to trap these inert gases). Note as well that radioxenon is released from medical isotope production facilities and these emissions interfere with national Data Centers' ability to monitor for nuclear testing in support of the Comprehensive Nuclear Test Ban Treaty. Therefore, the use of the silicate cages will also prove beneficial to the mitigation of the release of these isotopes. Other potential

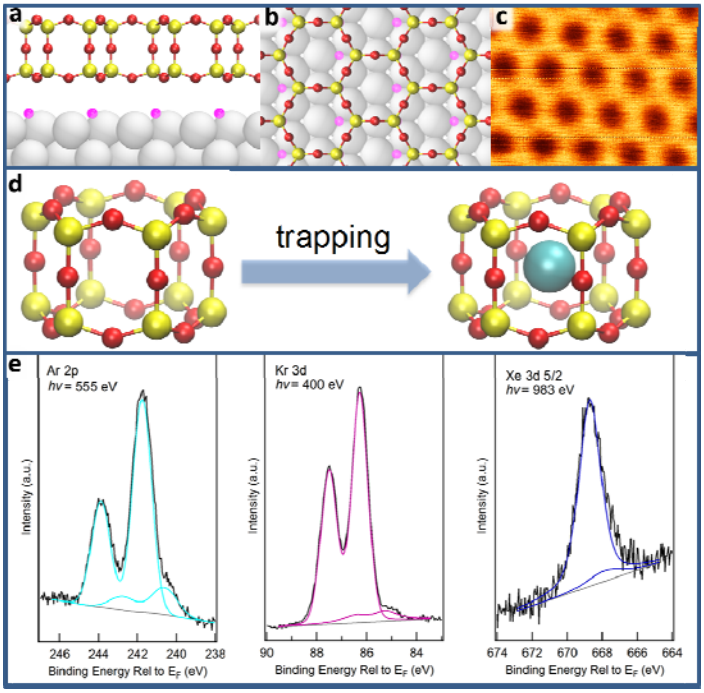

Figure 1. ***a*** and ***b*** show side and top views of the nano-porous aluminosilicate material proposed for trapping radiological noble gases. ***c*** shows a scanning tunneling microscopy image of the hexagonal structure of the material, the distance between hexagons is 0.55 nm. ***d*** depicts a cage of the material before and after trapping a single atom of the noble gas. ***e*** shows XPS spectra of noble gases trapped in these cages including the Ar 2p, Kr 3d, and Xe $3d_{5/2}$ core levels.

applications in photocathodes and photodetectors have been identified in conversations with the instrumentation division, which are not explicitly included as part of this proposal but could also benefit from this research.

It is worth noting that metal organic frameworks (MOFs) have been proposed for similar applications by other researchers at PNNL.[5] We have discussed a potential collaboration with Dr. Praveen Thallapally at PNNL in relation to testing MOFs at the BNL facilities and identified the possibility of future DTRA funding. The advantages of the proposed silicate materials include higher thermal stability (>1200 K) and higher resistance to radioactive damage than fragile metal-organic structures. Additionally, the proposed materials are made of some of the most abundant elements in the earth's crust (Si, Al, and O), giving the potential of a much lower cost of production compared to MOFs if future applications stem from this research.

Table 1. Experiment Matrix

	Non-radioactive isotopes	Radioactive isotopes
Silicate nanosheet on Ru(0001)	✓	✓
POSS nanocages on Ru film	✓	✓
HAS-1 Material (SBA-15)	✓	✓
HAS-2 Material (metal sponge)	✓	✓

The experiments proposed here, briefly summarized in table 1, aim at fundamental studies to assess the trapping of radiological noble gases in these cages at relevant concentrations and conditions. While the feasibility data for this LDRD was obtained in the context of internal research, the additional *inter-directorate* research needed for this *moderate risk-high reward* project requires LDRD funding. Such resources will permit sufficient data collection to develop a solid proposal to request external funding. Examples of this external funding include DOE Early Career Award (*Sanders*), DOE NA-22, DOE Isotope Program, DOD opportunities, as well as the NIH.

The research will focus on the trapping of three gases: Kr, Xe, and Rn, at conditions relevant to the potential applications described above. The proposal will start with two parallel activities. The design and construction of the experimental setup for the measurements with radioactive gases, to be carried out at the Medical Isotope Research & Production (MIRP), where the proposed research falls within the current safety envelope of the facility. In parallel, we will plan experiments at Argonne National Lab (ANL), to trap radioactive Kr or Xe, and follow the exponential decay using Gammasphere, which has about 100 Ge detectors. Concomitantly, we will start carrying out experiments with non-radioactive gases in air mixtures with relevant concentrations of noble gases (except for Rn) at the CFN and NSLS-II. These concentrations will vary between 1 and 500 ppmv (parts per million by volume). *In situ* trapping experiments will be carried out at pressures up to 10 Torr (max. pressure at AP-XPS instruments at CFN and NSLS-II), and *ex situ* following exposure to atmospheric pressure. Mixtures of noble gases will be used to assess selectivity. For the initial experiments, we will use silicate nanosheets (line 1 in experimental matrix) that we have already tested at the CFN for trapping pure noble gases at low pressures.[4] Therefore preliminary studies have shown that the silicate nanosheet are capable of

trapping nonradioactive gases on the order of 1 nmol/cm^2. For reference, studies with radioactive gases will involve concentrations in the picomolar range for the entire study. A second material to test is based polyoctahedral silsesquioxanes ("POSS") nanocages deposited on metal films. In recent experiments (unpublished) we have shown that these also trap noble gases. In parallel, we will work on the synthesis of higher surface area (HAS) materials that can be potentially scaled up, based on the deposition of POSS cages on nanoporous supports. These two prospective materials, HSA-1 and HSA-2, will use SBA-15 silicates and metal sponges as high surface area supports, respectively. These HSA trapping materials will be tailored for each specific application, depending on the need or higher surface areas, or specific form or shapes (monoliths vs. films vs powders). Trapping experiments will be carried out initially at room temperature, and the thermal stability of the gases in the cages will be assessed after trapping. Preliminary data obtained by XPS at NSLS-II has shown that the trapped gases are stable in the cages even after returning to UHV conditions at 300 K. Upon heating in UHV, Kr desorbs from the cages at 523 K and Xe at 723 K. Rn is predicted to desorb at 773 K, based on DFT calculations.[4] Further, **Figure 2** shows the potential trapping mechanism for the ions, as well as the experimental and simulated data on the kinetics of trapping Xe.

The proposed research seeks to utilize the Brookhaven Linac Isotope Producer (BLIP) at BNL to co-produce ^{211}Rn during the production of ^{225}Ac. Isolation of ^{211}Rn on a solid-state support, which subsequently decays to ^{211}At, can be transported to other locations or can be used to directly produce ^{211}At. We will exploit the co-produced material by trapping and harvesting the volatilized radon to act as a source of ^{211}At. ^{211}Rn is a radioactive noble gas with a half-life of 14.6 hours, which decays via two pathways, the first being a 27.4% alpha emission to stable ^{207}Po and second being a branching ratio of 76.4% decay via electron capture to ^{211}At. Employing the chemical differences between inert noble gases, halogens, and metals could provide for facile separations, thus providing a carrier-free source of ^{211}At for radiopharmaceutical applications. The experimental setup for radiological measurements will be built at the MIRP facility, experiments will be performed under the same experimental conditions described above. The determination of trapping of the radioactive isotopes will be based on gamma spectroscopy measurements. The isotopes to be used have a relatively short half-life and will decay to safe concentrations within a reasonable time frame (weeks), so radioactive waste will not remain passed

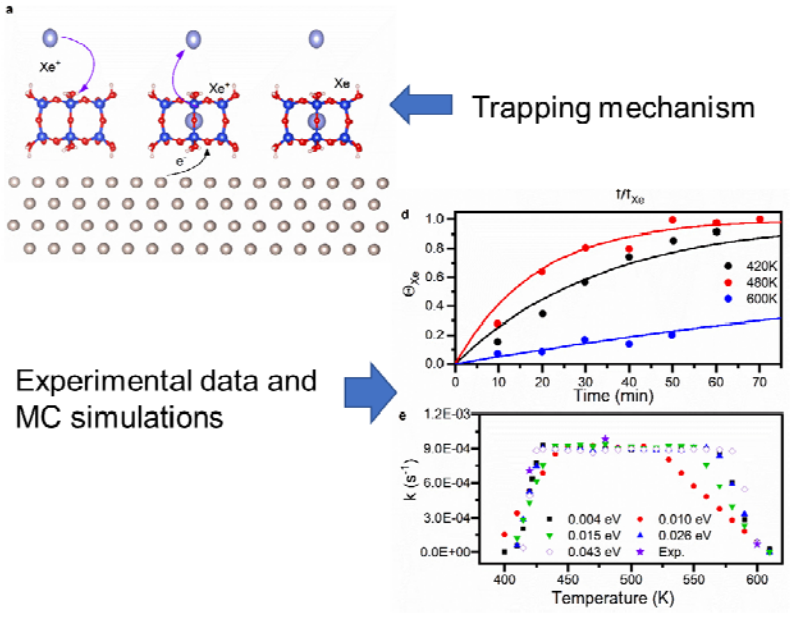

Figure 2. Top: diagram showing the trapping mechanism, in which a noble gas ion enters the silicate cage, gets neutralized by an electron from the metal support, and stays trapped in the neutral state. Bottom-right, experimental and simulated data on the kinetics of trapping Xe in nanocages, including change in coverage as a function of time trapping rate constracts obtained from such data.

the period of the LDRD. In the initial studies the silicate cages will be evaluated for their ability to trap xenon and radon independently from air mixtures. We will optimize the form and amount of material used to trap the gases as necessary. We will then evaluate the selective trapping of the radioactive gases from mixed gas systems, simulating target dissolution processes. Finally, in the case of radon trapping we will evaluate various solvent systems to be used for the removal of astatine-211 (from the decay of Rn-211) to develop a radioisotope generator for the production of At-211. We will also assess the reusability of the silicate cages during these studies.

As new/improved forms of the materials are developed during the project, experiments will be carried out on these new materials, using both radioactive isotopes at the MIRP setup and at ANL, and non-radioactive ones at the CFN and NSLS-II. A summary of the timeline is included below.

While this project carries moderate risk and the proposed experiments are needed to clearly assess the application potential, preliminary data suggests the benefits greatly outweigh the risks, given the new research areas that will stem from this project and the potential in-house development of intellectual property related to energy, medical applications, fundamental nuclear science, and national security.

Date	Objectives
6 Months	Synthesis of bilayer silicates and new high-surface area materials. Experiments of air mixtures including non-radioactive noble gases at conditions relevant to nuclear energy, non-proliferation, and medical isotopes production, using the single layer silicates as traps at the CFN and NSLS-II.
12 Months	Design and construction of an experimental setup at the MIRP facility for capture experiments using radioactive gases. Experiments at the CAlifornium Rare Isotope Breeder Upgrade (CARIBU) facility at Argonne National Laboratory Trapping experiments with high surface area materials at the CFN (non-radioactive gases).
18 Months	Start experiments with air mixtures, including radiological noble gases at relevant concentrations at the MIRP instrument.
24 Months	Analyze and publish results and patents. Carry out experiments with both radioactive and non-radioactive gases using as traps porous silicates: (1) a powder with accessible pores and (2) single- or few-layer films.
36 Months	Analyze and publish results and patents. Refine experiments to optimize materials and conditions for trapping noble gases. Summarize results of LDRD and plan future directions. Apply for external funding and/or license newly discovered trapping materials to obtain funds to continue research.

References

1 Zhong, J.-Q. *et al.* Immobilization of single argon atoms in nano-cages of two-dimensional zeolite model systems. *Nat Commun* **8**, 16118, doi:10.1038/ncomms16118 (2017).

2 Boscoboinik, J. A. & Shaikhutdinov, S. Exploring Zeolite Chemistry with the Tools of Surface Science: Challenges, Opportunities, and Limitations. *Catalysis Letters* **144**, 1987-1995, doi:10.1007/s10562-014-1369-3 (2014).

3 Boscoboinik, J. A., Yu, X., Yang, B., Shaikhutdinov, S. & Freund, H.-J. Building blocks of zeolites on an aluminosilicate ultra-thin film. *Microporous Mesoporous Mater.* **165**, 158-162, doi:10.1016/j.micromeso.2012.08.014 (2013).

4 Ionization-Facilitated Formation of Two-Dimensional (Alumino)silicate-Noble Gas Clathrate Compounds. J.-Q. Zhong, M. Wang, N. Akter, J.D. Kestell, T. Niu, A.M. Boscoboinik, T. Kim, D.J. Stacchiola, Q. Wu, D. Lu, J.A. Boscoboinik. *Adv. Funct. Mater*. 2019, DOI:10.1002/adfm.201806583

5 Chen, L. *et al.* Separation of rare gases and chiral molecules by selective binding in porous organic cages. *Nat Mater* **13**, 954-960, doi:10.1038/nmat4035 (2014).

VITA
Vanessa A. Sanders

Position/Title: Assistant Scientist, Medical Isotope Research & Production Program, Collider-Accelerator Department, Brookhaven National Laboratory

Education and Training:

B.A., Chemistry, Florida Memorial University, 2009, Miami Gardens, Florida

Ph.D., Radiochemistry, University of Nevada Las Vegas, 2017, Las Vegas, Nevada

Research and Professional Experience:

2019-present Assistant Scientist, Medical Isotope Research and Production Brookhaven National Laboratory. Routinely performed separations and radioanalytical analyses on medically relevant radioisotopes including ^{72}As, ^{177}Lu, ^{67}Cu, $^{44/47}$Sc, ^{225}Ac, and ^{227}Th.

2017-2019 Postdoctoral Fellow, Medical Isotope Research and Production Brookhaven National Laboratory.

Publications:

1. **Vanessa A. Sanders,** Edwin C. Pratt, Dinesh Bhupathiraju, Jason Lewis, Lynn Francesconi, Cathy Cutler. ^{227}Th Labeled 3,4,3-(LI-1,2-HOPO): Optimized Synthesis, Biological Distribution and Dosimetry. JNM Supplemental
2. Hatcher-Lamarre, J. L.; **Sanders, V**. A.; Rahman, M.; Cutler, C. S.; Francesconi, L. C., Alpha emitting nuclides for targeted therapy. *Nuclear Medicine and Biology* **2021,** *92*, 228-240
3. Phipps, M. D.; **Sanders, V. A**.; Deri, M. A., Current State of Targeted Radiometal-Based Constructs for the Detection and Treatment of Disease in the Brain. *Bioconjug.Chem.* **2021**.
4. **Sanders, V. A**.; Cutler, C. S., Radioarsenic: A promising theragnostic candidate for nuclear medicine. *Nuclear Medicine and Biology* 2021, *92*, 184-201.
5. **Sanders, V.A**.; et. al. ^{99m}Tc and ^{188}Re Pretargeting SPECT and Radioimmunotherapy Imaging Agents Employing Bioorthogonal Diels-Alder Click Chemistry. *In Preparation*
6. **Sanders, V.A**.; Cutler, C.S., Chelators for Theragnostic Agents. *In Preparation.*
7. Lukas, C. M.; Kesner, A.; Pratt, E. C.; **Sanders, V. A.;** et. al. The Impact of Positron Range on PET Resolution, Evaluated with Phantoms and PHITS Monte Carlo Simulations for Conventional and Non-conventional Radionuclides. *Mol Imaging Biol* **22,** 73–84 (2020).
8. **Sanders, V. A.;** Gao, M.; Turkman, N.; Kim, J.; Cutler C.S. Synthesis, Stability and In Vivo Imaging of the Indirect Incorporation of Arsenic- 72 on Therapeutic Antibodies, Nucl Med Biol., 2019, 72-73, S45-S46
9. **Sanders, V. A.;** Iskhakov, D.; Abdel-atti, D.; Devany, M.; Neary, M.C.; Czerwinski, K.R.; Francesconi, L.C., Synthesis, characterization, and biological studies of rhenium, technetium-99m, and rhenium-188 pentapeptides. *Nuclear Medicine and Biology* 2019, 68-69, 1-13

Invited Presentations

Fall 2020 APS-DNP Annual Meeting, The Development of PET Generator Systems at the Brookhaven Linac Isotope Producer

Spring 2020 SNMMI Annual Meeting, Radiolabeling Comparison of Accelerator Versus Generator Produced ^{225}Ac

Fall 2019 Georgia State University Colloquium, The Production of Medical Isotopes Using the Brookhaven Linac Isotope Producer

Honors and Fellowships

2021 2021 Own Your Excellence Award- Florida Memorial University

2020 Society of Nuclear Medicine and Molecular Imaging Future Leader

2019 Science and Technology in Society Forum Young Leader

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Education & Training

University of Washington, Seattle, WA	Ph.D.	1997	Physics
Argonne National Laboratory, Argonne, IL	Postdoc	1997-1999	Nuclear Physics

Research & Professional Experience

Brookhaven National Laboratory Since August 1999
Physicist
Currently Nuclear Science and Technology Department Chair since January 1st, 2021, www.bnl.gov/nst

Selected Publications relevant to current proposal

The Plutonium Handbook 2nd edition, Volume 1, Chapter 3, Plutonium Nuclear Science
M.B. Chadwick, P. Moller, E. Lynn, A.A. Sonzogni
American Nuclear Society, published 2019, http://www.ans.org/pubs/handbooks/plutonium/

Dissecting Reactor Antineutrino Flux Calculations
A.A. Sonzogni, E.A. McCutchan, and A.C. Hayes
Phys. Rev. Lett. **119**, 112501 (2017).

Effects of Fission Yield Data in the Calculation of Antineutrino Spectra for ^{235}U(n,fission) at Thermal and Fast Neutron Energies
A.A. Sonzogni, E.A. McCutchan, T.D. Johnson, and P. Dimitriou
Phys. Rev. Lett. **116**, 132502 (2016).

γ-ray Fluxes in Oklo Natural Reactors
C.R. Gould, E.I. Sharapov, A.A. Sonzogni
Phys. Rev. C **86**, 054602 (2012).

Reactor Decay Heat in ^{239}Pu: Solving the γ Discrepancy in the 4-3000-s Cooling Period
A. Algora, *et al*.
Phys. Rev. Lett. **105**, 202501 (2010).

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Jorge **Anibal** Boscoboinik

POSITION TITLE & INSTITUTION: Materials Scientist, Brookhaven National Laboratory

Institution	Location	Major/Area of Study	Degree (if applicable)	Year YYYY
Fritz-Haber Institute of the Max-Planck Society	Berlin, Germany	Physical Chemistry	Postdoc	2013
University of Wisconsin, Milwaukee	Milwaukee, WI	Physical Chemistry	PhD	2010
Universidad Nacional de San Luis	San Luis Argentina	Chemistry	BSc	2005

APPOINTMENTS

10.01.2018 – current	**Materials Scientist.** Center for Functional Nanomaterials. Brookhaven National Laboratory. Upton, NY, United States.
10.01.2015 – 09.30.2018	**Associate Materials Scientist.** Center for Functional Nanomaterials. Brookhaven National Laboratory. Upton, NY, United States.
10.07.2013 – 09.30.2015	**Assistant Materials Scientist.** Center for Functional Nanomaterials. Brookhaven National Laboratory. Upton, NY, United States.
03.01.2011 – 9.30.2013	**Alexander von Humboldt Postdoctoral Fellow.** Fritz-Haber Institute of the Max Planck Society.
08.15.2005 – 01.15.2011	**Teaching and Research Assistant**. University of Wisconsin Milwaukee. Milwaukee, WI, United States.
02.01.2005 – 07.31.2005	**Quality and Development Analyst**. Kimberly Clark Corp. Buenos Aires, Argentina.

Selected Publications (complete list here)

1. Ionization-Facilitated Formation of Two-Dimensional (Alumino)silicate-Noble Gas Clathrate Compounds. J.-Q. Zhong,M. Wang, N. Akter, J.D. Kestell, T. Niu, A.M. Boscoboinik, T. Kim, D.J. Stacchiola, Q. Wu, D. Lu, **J.A. Boscoboinik.** *Adv. Funct. Mater.* **2019**, DOI:10.1002/adfm.201806583

2. Immobilization of single argon atoms in nano-cages of two-dimensional zeolite model systems. J.-Q. Zhong, M. Wang, N. Akter, J.D. Kestell, A.M. Boscoboinik, T. Kim, D. J. Stacchiola, D. Lu, **J.A. Boscoboinik.** *Nat. Commun.* **2017**, DOI: 10.1038/ncomms16118

3. Room-Temperature in Vacuo Chemisorption of Xenon Atoms on Ru(0001) under Interface Confinement. J.-Q. Zhong, M. Wang, N. Akter, D.J. Stacchiola, D. Lu, **J.A. Boscoboinik**
J. Phys. Chem. C **2019**, DOI: 10.1021/acs.jpcc.9b01110.

4. J.A. Boscoboinik*: Chemistry in confined space through the eyes of surface science—2D porous materials. *J. Phys.: Condens. Matter* **2019**, 31, 063001, DOI: 10.1088/1361-648X/aaf2ce.

5. Mechanism of the Accelerated Water Formation Reaction under Interfacial Confinement.
M. Wang, C. Zhou, N. Akter, W.T. Tysoe, **J.A. Boscoboinik**, D. Lu.
ACS Catal. **2020**, DOI: 10.1021/acscatal.9b05289

(a) SYNERGISTIC ACTIVITIES

1. Guest Editor, Special Issue in Springer journal "Topics in Catalysis", in 2019.
2. Co-organizer of workshops at the CFN-NSLS-II users' meeting in 2015 and 2018.
3. General organizer of the San Luis International Conference and Summer School on Surface Science and Heterogeneous Catalysis. www.surfacecatalysis.org
4. Founder of the Surface Science Network in 2009. An initiative aiming to create an interactive community among people that work in fields related to surface science. Website: www.surfacesciencenetwork.com
5. Reviewer for: J. Am. Chem. Soc., Angew. Chem., Rev. Sci. Inst., Catal. Lett., J. Phys. Chem. C., Catal. Today., J. Phys. Chem. Lett., Top. Catal., Micropor. Mesopor. Mater., Surf. Sci., Physica A, ACS Catal., Nat. Commun., etc

1. EQUIPMENT (Reference: DOE Order 413.2C for guidance on equipment restrictions)

Will LDRD funding be used to purchase equipment? **N**

If "Yes," provide cost and description of equipment
Year 1 - $

Year 2 - $

Year 3 - $

Description:

2. HUMAN SUBJECTS (Reference: DOE Order 443.1)

Are human subjects involved from BNL or a collaborating institution? Human Subjects is defined as "A living individual from whom an investigator obtains either (1) data about that individual through intervention or interaction with the individual, or (2) identifiable, private information about that individual".

If **yes**, attach copy of the current Institutional Review Board Approval and Informed Consent Form from BNL and/or collaborating institution. **N**

3. VERTEBRATE ANIMALS

Are live, vertebrate animals involved? **N**

If **yes**, attach copy of approval from BNL's Institutional Animal Care and Use Committee. **N/A**

4. NEPA REVIEW

Are the activities proposed similar to those now carried out in the Department/Division which have been previously reviewed for potential environmental impacts and compliance with federal, state, local rules and regulations, and BNL's Environment, Safety, and Health Standards? (Therefore, if funded, proposed activities would require no additional environmental evaluation.) **Y**

If **no**, has a NEPA review been completed in accordance with the National Environmental Policy Act (NEPA) and Cultural Resources Evaluations Subject Area and the results documented? **N/A**

(**Note:** If a NEPA review has not been completed, submit a copy of the work proposal to the BNL NEPA Coordinator for review. No work may commence until the review is completed and documented.)

5. ES&H CONSIDERATIONS

Does the proposal provide sufficient funding for appropriate decommissioning of the research space when the experiment is complete? **Y**

Is there an available waste disposal path for project wastes throughout the course of the experiment? **Y**

Is funding available to properly dispose of project wastes throughout the course of the experiment? **Y**

Are biohazards involved in the proposed work? If yes, attach a current copy of approval from the Institutional Biosafety Committee. **N**

Can the proposed work be carried out within the existing safety envelope of the facility (Facility Use Agreement, Nuclear Facility Authorization Agreement, Accelerator Safety Envelope, etc.) in which it will be performed? Y

If **no**, attach a statement indicating what has to be done and how modifications will be funded to prepare the facility to accept the work.

6. TYPE OF WORK Select Basic, Applied or Development **Development**

7. ALIGNMENT WITH THE LABORATORY PRIORITIES

This proposal is directly aligned with the Isotope Production and R&D Capabilities initiative as the utilization of the silicate cages which trap noble radioactive gases will allow for the mitigation of gaseous release during routine production of isotopes. Also, the silicates have the potential to lead to alternative production routes for medical isotopes through the indirect production of astatine-211. Further this proposal is aligned with the Nuclear Physics initiative as the data obtained during these studies will increase the fundamental understanding of decay chains that occur following nuclear detonation events. Finally, this proposal is also aligned with the Clean Energy and Climate initiative. More specifically, trapping Xe and Kr can increase the efficiency and safety of the new generation modular nuclear reactors currently under development and testing, contributing to the development of a clean and reliable source of energy. Additionally, trapping these gases in silicate materials, can contribute to controlling the emissions of radioactive gases from current and future nuclear waste sites.

8. POTENTIAL FUTURE FUNDING

Upon completion of this proposal, we intend to use the preliminary data to apply for funding from outside agencies such as the Department of Defense (DoD) and the National Institutes of Health (NIH) to assist in translating the use of the produced medical isotopes to preclinical studies. These awards typically range between $250 K and $500 K per year. We also intend to use the data for the application of an Early Career Award. Submissions to this opportunity would occur within 1 FY of the completion of this LDRD. Funding for each these opportunities are upwards of $500 K per year.

Other future funding opportunities include DOE nuclear energy division, and DOE Technology Commercialization Fund grants, to which data from this LDRD will contribute. In previous years, the awards for **both** of these opportunities were $1 M per year. We are currently in discussions with nuclear energy companies to evaluate forming partnerships to test this technology in new modular reactors.

9. BUDGET JUSTIFICATION

Labor

LDRD	Year 1		Year 2		Year 3	
Labor	FTEs	Amounts	FTEs	Amounts	FTEs	Amounts
SCI 1	0.15	26,687	0.25	45,851	0.25	48,072
Post Doc.	0.52	48,608	0.53	50,844	0.53	52,623
Grad Student	1.00	50,000	1.00	50,000	1.00	50,000

Vanessa A. Sanders: SCI 1. Dr. Sanders will serve as the Principal Investigator on this grant and will lead the proposed research including all experimentation, publications, and presentations of the results for the experiments that occur in the medical isotope production research facility. She will supervise the postdoc on this grant and co-supervise the graduate student on this project.

Post-doc: One post-doc covered at 50%. Their duties include the testing of the silicate cages, implementation of the trapping device, and extraction studies of daughter isotopes.

Graduate Student: A graduate student will be employed over a four-year period. Their duties will include the synthesis, characterization and functionalization of the aluminosilicate cages.

Materials

Total Funds Requested: Year 1-$75,000 Year 2-$55,000 Year 3-$55,000

Glove Box

Funds Requested: Year 1-$20,000

A glovebox will be purchased for $10,000. This glovebox will be used to conduct the initial experiments of testing the silicate cages with radioactive gases.

Isotopes
Funds Requested: Year 1-$40,000 Year 2-$40,000 Year 3-$40,000
Isotope will be purchased from National Isotope Development Center (NIDC) and Lantheus to test the silicate cages.

Misc. Materials
Funds Requested: Year 1-$10,000 Year 2-$10,000 Year 3-$10,000
These funds are requested to purchase specialty glassware, sample holders, gaskets, gases and other consumables.

Automation
Funds Requested: Year 1-$5,000 Year 2-$5,000 Year 3-$5,000
Automation System hardware will be purchased to automated the trapping device during target dissolution processes.

Travel
Funds Requested: Year 1-$6,500 Year 2-$6,500 Year 3-$6,500
Travel is requested to present the proposed research at international and national meetings. Examples of these meetings include the American Chemical Society, the International Symposium of Technetium and Other Radiometals in Chemistry and Medicine, the International Symposium on Radiopharmaceutical Sciences, the Society of Nuclear Medicine and Molecular Imaging, and the Targeted Alpha Therapy meetings.

ES&H Support Recharge
Funds Requested: Year 1-$5,000 Year 2-$5,000 Year 3-$5,000
The requested funds Radiological Support will be used to develop work permits, provide coverage for transferring samples, and provide work oversight.

Budget Justification for NE Directorate

Dr. Alejandro Sonzogni is also submitting a budget which will be requesting funds to cover a post-doc. Their duties include conducting the analyses of gases trapped in the silicate cages. These experiments will be conducted at the ANL Gammasphere. For this budget we are requesting the following.

Year 1- $ 75,000 Year 2- $ 75,000 Year 3- $ 75,000

10. NAME OF SUGGESTED BNL REVIEWERS

Cathy Cutler (C-AD)
Jack Shlachter

APPROVALS--NPP

Business Operations Manager

Susan M. Pankowski

Susan M. Pankowski

Department Chair/Division Manager

DocuSigned by:
Thomas Roser
BB1239D7FF004B9...

Thomas Roser

Associate Laboratory Director for
Nuclear and Particle Physics

Haiyan Gao

APPROVALS--EBNN

Business Operations Manager

Ken Koebel

Kenneth Koebel

Department Chair/Division Manager

Alejandro Sonzogni

Associate Lab Director/EBNN

Martin Schoonen

FY22 Budget Proposal
TRAPPING NOBLE GASES IN SILICATE NANOCAGES FOR MEDICAL ISOTOPES, NUCLEAR ENERGY, AND NUCLEAR NONPROLIFERATION
PI: Vanessa Sanders & Anibal Boscoboinik
($ in Whole Numbers)

R/C	Description	FY22 Year 1		FY23 Year 2		FY24 Year 3	TOTAL
100	Salaries	75,295		96,695		100,695	272,685
	Subtotal	**75,295**		**96,695**		**100,695**	**272,685**
	Total Labor	**75,295**		**96,695**		**100,695**	**272,685**
	Total Dist. Tech. Services	**-**		**-**		**-**	**-**
290	**Domestic Travel**	**6,500**		**6,500**		**6,500**	**19,500**
300	**PO Purchases**	**75,000**		**55,000**		**55,000**	**185,000**
	Total MST	**81,500.00**		**61,500**		**61,500**	**204,500**
	Total High-Value Procureme	**50,000**		**50,000**		**50,000**	**150,000**
	Departmental Org. Burdens	-	0.00%	-	0.00%	-	**-**
272	Departmental Org. Burdens	-	0.00%	-	0.00%	-	**-**
	Directorate Org Burdens	-	0.00%	-	0.00%	-	**-**
	Distributed Org. Burdens	**-**		**-**		**-**	**-**
637	ES&H Support Recharge	5,000		5,000		5,000	**15,000**
	Total ODC	**5,000.00**		**5,000**		**5,000**	**15,000**
	Total Power	**-**		**-**		**-**	**-**
	Total Cost (Excluding Overh	**211,795.00**		**213,195**		**217,195**	**642,185**
745	Procurement	9,205	7.00%	7,805	7.00%	7,805	**24,815**
	Total G&A	**-**	**0**	**-**	**11.30%**	**-**	**-**
	Project Total	**221,000**		**221,000**		**225,000**	**667,000**
	Full Cost Recovery	**-**	**-**	**-**	**0.00%**	**-**	**-**
	Sub Total	**221,000**		**221,000**		**225,000**	**667,000**
	Prior Year Carry Over	-		-		-	**-**
	Sub Total Project Funded Cc	**221,000**		**221,000**		**225,000**	**667,000**
	Expected Funding	-		-		-	**-**
	Total Authorized Funds (Nev	**221,000**		**221,000**		**225,000**	**667,000**
	Carry Forward	-		-		-	**-**
	Total Project Cost Plan	**221,000**		**221,000**		**225,000**	**667,000**

Brookhaven National Laboratory

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Directorate: *Environment, Biology, Nuclear Energy & Non Proliferation*
Department: *Nuclear Science & Tech Dept*
BudModID: *FY21_NE_LDRD_ALEJAND*
Principal Investigator: *SONZOGNI,ALEJANDRO A*
Sponsor: *BNL*
Project Rate Type: *NE LDRD*

Sum of Amount			Reporting Year			
Cost Type	Group Break Descr	Descr	2022	2023	2024	Grand Total
Direct Costs	BNL Direct Labor		$ 37,645	$ 37,645	$ 37,645	$ 112,934
	Departmental Charges	Electric - Distributed	$ 535	$ 535	$ 535	$ 1,604
		Infrastructure Charge-Distr	$ 4,009	$ 4,009	$ 4,009	$ 12,027
		Waste Mangement Alloc - Distr	$ 260	$ 260	$ 260	$ 779
		Special Org Burdens	$ 10,051	$ 10,051	$ 10,051	$ 30,153
	Departmental Charges Total		*$ 14,855*	*$ 14,855*	*$ 14,855*	*$ 44,564*
Direct Costs Total			$ 52,499	$ 52,499	$ 52,499	$ 157,498
Indirect Costs	Indirect Overheads-Project G&A	VAB Common Institutional Recov	$ 22,501	$ 22,501	$ 22,501	$ 67,502
	Indirect Overheads-Project G&A Total		*$ 22,501*	*$ 22,501*	*$ 22,501*	*$ 67,502*
Indirect Costs Total			$ 22,501	$ 22,501	$ 22,501	$ 67,502
Grand Total			$ 75,000	$ 75,000	$ 75,000	$ 225,000

Sum of FTE		Reporting Year			
LaborType	Name	2022	2023	2024	Grand Total
POST DOC	RA2 Post Doc TBD	0.38	0.37	0.36	1.10
Grand Total		0.38	0.37	0.36	1.10

Sum of Hours		Reporting Year			
LaborType	Name	2022	2023	2024	Grand Total
POST DOC	RA2 Post Doc TBD	689	671	651	2,011
Grand Total		689	671	651	2,011

Sum of Months		Reporting Year			
LaborType	Name	2022	2023	2024	Grand Total
POST DOC	RA2 Post Doc TBD	4.51	4.41	4.26	13.18
Grand Total		4.51	4.41	4.26	13.18