RESUME – Lindsay C. Shuller-Nickles

PERSONAL DATA

Assistant Professor
Department of Environmental Engineering and Earth Sciences
Clemson University
Anderson, SC 29625
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EDUCATION

Ph.D., University of Michigan, 2010, Materials Science and Engineering
Thesis title: "Atomistic Modeling of the Solid State Chemistry of Actinide Materials"
Advisor(s): Rodney Ewing and Udo Becker

M.S., University of Michigan, 2007, Materials Science and Engineering
B.S.E., University of Michigan, 2005, Materials Science and Engineering

PROFESSIONAL EXPERIENCE

Clemson University, 2011- , Assistant Professor of Environmental Engineering and Earth Science
University of Michigan, 2010-11, Postdoctoral Research Fellow of Geological Sciences, Advisor: Udo Becker

MEMBERSHIPS

Member, Association of Environmental Engineering and Science Professors, AEESP (2011-2012)
Member, American Chemical Society, ACS (2006-2007, 2011-)
Member, Materials Research Society, MRS (2006-)
Member, Mineralogical Society of America, MSA (2005-)

PROFESSIONAL ACTIVITIES

American Chemical Society, symposium chair, Young Investigators in Nuclear Chemistry and Technology (2016).
U.S. Department of Energy National Analytical Measurement Program (NAMP) Training and Education Committee, organizer of Nuclear Forensics webinar series (2015-).
U.S. Department of Energy National Analytical Measurement Program (NAMP) Training and Education Committee, member and guest lecturer (2013-).
Goldschmidt 2013 Conference, organizing team member, Select thematic sessions (2011-2013).

PUBLICATIONS

Refereed Journal Publications

Wen, Y., Xu, Y., Brinkman, K., and Shuller-Nickles, L. 2016. Cation ordering and phase stability in Cs-substituted $Ba_{1.33}Zn_{1.33}Ti_{6.67}O_{16}$, $Ba_{1.33}Ga_{2.66}Ti_{5.67}O_{16}$ and $Ba_{1.33}Al_{2.66}Ti_{5.33}O_{16}$ hollandite. *Scientific Reports*, **in review**.

Xu, Y., Grote, R., Wen, Y., Amoroso, J., Shuller-Nickles, L., Brinkman, K. 2016. A-site compositional effects in Ga-doped hollandite materials of the form $Ba_xCs_yGa_{2x+y}Ti_{8-2x-y}O_{16}$: implications for Cs immobilization in crystalline ceramic waste forms. *Scientific Reports*, **6**, Article number: 27412.

Xu, Y., Feygenson, M., Page, K., Shuller-Nickles, L., Brinkman, K. 2016. Structural Evolution in Hollandite Solid Solutions Across the A-site Compositional Range from $Ba_{1.33}Ga_{2.66}Ti_{5.34}O_{16}$ to $Cs_{1.33}Ga_{1.33}Ti_{6.67}O_{16}$. *Journal of the American Ceramic Society*, doi:10.1111/jace.14443.

Xie, Y., Helvenston, E.M., Shuller-Nickles, L.C. and Powell, B.A. 2016. Surface complexation modeling of Eu(III) and U(VI) interactions on graphene oxide. *Environmental Science and Technology*, **50**, 1821-1827.

Renock, D., and Shuller-Nickles, L. 2015. Predicting geologic corrosion with electrodes. *Elements*, **11**, 331-336.

Shuller-Nickles, L.C., Bender, W., Walker, S, and Becker. U. "Quantum-mechanical methods for quantifying incorporation of contaminants in proximal minerals." *Minerals*, **4**, 690-715 (2014).

Shuller, L.C., Ewing, R.C., and Becker, U. "Np-incorporation into uranyl phases: A quantum-mechanical evaluation," *Journal of Nuclear Materials*, **434**, 440-450 (2013).

Shuller-Nickles, L.C., Ewing, R.C., and Becker, U. "Atomistic calculations of the thermodynamic properties of mixing for tetravalent metal dioxide solid solutions: (Zr, Th, Ce)O_2," *Journal of Solid State Chemistry*, **197**, 550-559 (2013).

Shuller, L.C., Ewing, R.C., and Becker, U. "Thermodynamic properties of $Th_xU_{1-x}O_2$ ($0 < x < 1$) based on quantum-mechanical calculations and Monte-Carlo simulations," *Journal of Nuclear Materials*, **412**, 13-21 (2011).

Shuller, L.C., Ewing, R.C., and Becker, U. "Quantum-mechanical evaluation of Np-incorporation into studtite," *American Mineralogist*, **95**, 1151-1160 (2010).

Zhang, F., Pointeau, V., Shuller, L.C., Reaman, D.M., Lang, M., Lui, Z., Hu, J., Panero, W.R., Becker, U, Poinssot, C., and Ewing, R.C., "Structural transitions and electron transfer in coffinite, $USiO_4$, at high pressure," *American Mineralogist*, **94**, 916-920 (2009).

Skomurski, F.N., Shuller, L.C., Ewing, R.C., and Becker, U. "Corrosion of UO_2 and ThO_2: A quantum-mechanical investigation," *Journal of Nuclear Materials*, **375**, 290-310 (2008).

<u>Conference Proceedings</u> (Reviewed)

Y. Xu, Y. Wen, R. Grote, L. Shuller-Nickles, K. Brinkman, "Development of Ga Doped Hollandites for Cs Immobilization" in the 11th International Conference on Ceramic Materials & Components for Energy & Environmental Applications, American Ceramic Society (2016).

Pinder-Grover, T., Millunchick, J.M., Bierwert, C., and Shuller, L. "The efficacy of screencasts on diverse students in a large lecture course," *Proceedings of the*

American Society of Engineering Education, American Society of Engineering Education, Austin, Texas (June 2009).

Pinder-Grover, T., Millunchick, J.M., Bierwert, C., and Shuller, L. "Leveraging screencasts to strategically clarify unclear materials science concepts," *Proceedings of the American Society of Engineering Education*, American Society of Engineering Education, Austin, Texas (June 2009).

Shuller, L.C., Pavenayotin, N., Ewing, R.C., and Becker, U. "Thermodynamic properties of actinide dioxide solid solutions," *Materials Research Society Conference Proceedings*, Materials Research Society, Boston, MA (November, 2008).

Shuller, L.C., Pavenayotin, N., Skomurski, F.N., Ewing, R.C., and Becker, U. "Thermodynamic properties of actinide-zirconium dioxide solid-solutions relevant for advanced nuclear fuels," *Waste Management 2008 Conference Proceedings*, Pheonix, AZ (March 2008).

Shuller, L.C., Ewing, R.C., and Becker, U. "Np incorporation into K-boltwoodite," *Materials Research Society Conference Proceedings*, Materials Research Society, Sheffeld, UK (August 2007).

Shuller, L.C., Ewing, R.C., and Becker, U. "Np incorporation into uranyl alteration phases: A quantum mechanical approach," *Materials Research Society Conference Proceedings*, Materials Research Society, Boston, MA (November, 2006).

Research Reports

Eaton, G.F., Genetti, V., Hu, Q., Hudson, G.B., Kersting, A.B., Lindvall, R.E., Moran, J.E., Nimz, G.J., Ramon, E.C., Rose, T.P., Shuller, L.C., Williams, R.W., Zavarin, M., Zhao, P. "Hydrologic Resources Management Program and Underground Test Area Project FY2005 Progress Report," Lawrence Livermore National Laboratory, *UCRL-TR-229708*, (March, 2007).

PRESENTATIONS

Hoover, M. and Shuller-Nickles, L. "Divalent Cation Incorporation into Actinide Oxides," American Chemical Society, Philadelphia, PA (August 2016).

Hoover, M., Buff, J., Earle, M., Earnhart, J., Wyant, P, and Shuller-Nickles, L. "Coupling Experiments and Atomistic Modeling to Characterize Actinide Oxides in Support of Nuclear Forensics," Nuclear Forensics Academic Laboratory Collaborations Meeting, Argonne, Illinois (August 2016).

Merritt, E. and Shuller-Nickles, L. "Evaluation of an Aqueous Phase Derivatization Reaction of Acetohydroxamic Acid," Hydrogeology Symposium, Clemson, SC (March 2016).

Earnhart, J. and Shuller-Nickles, L. "Evaluation of Elemental Distribution in Trinitite Using Electron Microscopy," Hydrogeology Symposium, Clemson, SC (March 2016).

Buff, J. and Shuller-Nickles, L. "Quantum-mechanical calculations of iodine incorporation into $Ag(NO_3)$," American Chemical Society, San Diego, CA (March 2016).

Shuller-Nickles, L. "Uranium Resources," invited webinar for the U.S. Department of Energy's National Analytical Management Program (NAMP) (January 2016).

Shuller-Nickles, L. "Advances in Incorporation Energy Calculations," Geological Society of America, Baltimore, MD (November 2015).

Hoover, M. and Shuller-Nickles, L. "Divalent cation incorporation into UO_2 and PuO_2," Geological Society of America, Baltimore, MD (November 2015).

Wen, Y., Hood, D., Renock, D., Shuller-Nickles, L. "Changes to Uranium Redox Processes Due to Sorption onto or Incorporation into Fe-bearing minerals," Radionuclide Migration, Santa Fe, New Mexico (September 2015).

Shuller-Nickles, L., Young, S., Seliman, A., Bliznyuk, V., and DeVol, T. "Time-dependent density functional theory calculations to guide the development of modified organic scintillating materials," Radiobioassay and Radiochemical Measurement Conference, Knoxville, TN (October 2014).

Helvenston, E.M., Chatman, A., Powell, B.A., Shuller-Nickles, L.C., "Ab Initio Calculations and Experimental Studies of Uranyl Sorption to Graphene Oxide," American Chemical Society Conference, San Francisco, California (August 2014).

Shuller-Nickles, L. "Coupling Experiments and Atomistic Modeling to Characterize Actinide Oxides in Support of Nuclear Forensics," Nuclear Forensics Academic Laboratory Collaborations Meeting, Argonne, Illinois (August 2014).

Shuller-Nickles, L. "Materials Science of Uranium (and how it can be used for nuclear forensics)," invited talk for the Nuclear Forensics Summer School, Columbia, Missouri (July 2014).

Hood, D., Shuller-Nickles, L., "pH Mediated Redox Behavior of Uranium Incorporated into Hematite,"American Chemical Society Conference, Dallas, Texas (March 2014).

Shuller-Nickles, L. "Integrated computational and experimental study of Fe-oxide minerals as getters for uranium," invited talk for University of Georgia Geology Department, Athens, Georgia (November 2013).

Wen, Y., Renock, D., Shuller-Nickles, L., "Role of Fe(II) on Actinide Redox Processes at Mineral Surfaces," Radionuclide Migration, Brighton, United Kingdom (September 2013).

Hood, D., Wen, Y., Shuller-Nickles, L., "Redox Behavior of Uranium Incorporated into Hematite,", Goldschmidt Conference, Florence, Italy (August 2013).

Wen, Y., Renock, D.R., Shuller-Nickles, L., "Actinide Redox on Semiconducting Mineral Surfaces," 12^{th} International Conference on the Biogeochemistry of Trace Elements," Athens, Georgia (June 2013).

Shuller-Nickles, L., "Molecular Modeling of Radioactive Contaminants in the Environment," invited (by Jim Bottum) for Clemson University CITI exhibit at Supercomputing Conference, Salt Lake City, UT (November 2012).

Shuller-Nickles, L., "Using Molecular Modeling to Study the Fate of Radioactive Contaminants in the Environment," invited talk for Clemson University Environmental Toxicology Program, Clemson, SC (April 2012).

Shuller-Nickles, L., "Quantum-mechanical calculations and Monte Carlo simulations of the thermodynamic mixing properties for tetravalent AO_2 (A = Zr, Ce, Th, U)," invited talk for Georgia Institute of Technology, Atlanta, GA (October 2011).

Shuller-Nickles, L., "Quantum-mechanical calculations and Monte Carlo simulations of the thermodynamic mixing properties for tetravalent AO_2 (A = Zr, Ce, Th, U)," invited talk for University of South Carolina, Columbia, SC (October 2011).

Shuller-Nickles, L., Renock, D., Rak, Z., Fernando, S., Dzulkifli, I., Ewing, R.C., and Becker, U., "Actinide adsorption onto mineral surfaces: A quantum-mechanical investigation," American Chemical Society, Denver, CO (September 2011).

Becker, U., Shuller-Nickles, L., Rak, Z., and Ewing, R. "Actinide incorporation into uranyl minerals and garnets," American Chemical Society, Denver, CO (August 2011) invited talk – presented as substitute.

Shuller, L.C., Ewing, R.C., and Becker, U., "Quantum-mechanical evaluation of Np-incorporation into studtite," American Nuclear Society, Las Vegas, NV (November 2010).

Shuller, L.C., "Calculating the solid state chemistry of nuclear materials: From nuclear fuel development to nuclear waste management," invited talk for National Institute of Standards and Technology, Gaithersburg, MD (February 2010).

Shuller, L.C., Ewing, R.C., and Becker, U., "Actinide incorporation and sorption in layered structures," Integrated Radioactive Waste Management for Future Fuel Cycles, Charleston, SC (October 2009). (Poster)

Shuller, L.C., Ewing, R.C., and Becker, U., "Computational investigation of the thermodynamic mixing properties of actinide dioxide solid solutions," Materials Science and Technology, Pittsburgh, PA (October 2009).

Shuller, L.C., Poling, J., Ewing, R.C., and Becker, U., "Quantum-mechanical calculations of aqueous actinide adsorption onto hematite (001)," Radionuclide Migration, Kennewick, WA (September 2009). (Poster)

Shuller, L.C., Poling, J., Ewing, R.C., and Becker, U., "Actinide adsorption onto hematite (001) surface," Goldschmidt, Vancouver, British Columbia (July 2008). (Poster)

Shuller, L.C., Ewing, R.C., and Becker, U., "Computational investigation of Np incorporation into K-boltwoodite," American Chemical Society, Chicago, IL (March 2007).

Shuller, L.C., Ewing, R.C., Becker, U., "Np^{5+} incorporation into uranyl alteration phases: a quantum mechanical approach," American Geophysical Union Joint Meeting, Baltimore, MD (May 2006) (Poster)

HONORS AND AWARDS

First Place in Innovations in Fuel Cycle Research student paper competition, United States Department of Energy (2010).

Best Student Poster, Integrated Radioactive Waste Management for Future Fuel Cycles Conference (2009).

Best Poster in session, Waste Management Conference (2008)

Office of Civilian and Radioactive Waste Management Fellowship, United States Department of Energy (2007-2010).

Roy G Post Scholarship, Post Foundation (2007)
Marion Sarah Parker Scholars, University of Michigan College of Engineering (2004)

SPONSORED RESEARCH

"Energize: An Interactive Evaluation Tool for Engaging the General Public with Energy Decision Making," Dept. of Energy, PI (34%). $786,999 ($267,580), (2016-2019).

"High Temperature Melt Solution Calorimeter: The Thermodynamic Characterization of Oxides in Nuclear Energy," Dept. of Energy, co-PI (17.5%), $325,000 ($56,875), (2015-2016).

"Radionuclide Waste Disposal: Development of Multi-scale Experimental and Modeling Capabilities," Dept. of Energy, co-PI (5%), $5,250,000.00, ($262,500), (2014-2017).

"Coupling Experiments with Atomistic Modeling to Characterize Actinide Oxides in Support of Nuclear Forensics," Dept. of Homeland Security and Domestic Nuclear Detection Office (via SCUREF), PI, $382,433, ($382,433), (2014-2017).

OTHER SPONSORED ACTIVITY

"Two-Day Workshop at SRS," SCUREF, PI (100%), $18,700 ($18,700)**,** (2016-2017).

"Renewal REU Site: Interfaces and Surfaces," NSF, co-PI (3.3%), $201,666 ($6,655), (2015-2018).

"Clemson University Nuclear Engineering and Radiological Sciences Scholarship Program," Nuclear Regulatory Commission, PI (75%), $200,000, ($150,000), (2014-2018).

"Nuclear Energy and the Environment K-12 Educator Workshop", Clemson Environmental Institute, $6,500, (2011-2012).

"Early Career Geoscience Faculty Workshop Travel Grant", National Association of Geoscience Teachers, $400 (2012).

GRADUATE STUDENT ADVISING

Current Graduate Advising

Nichols, N.J., (M.S.), "Time-dependent density functional theory investigation of organic scintillating molecules," May 2017, (Advisor).

Wen, Y., (Ph.D.), "Elucidating the role of mineral surfaces on actinide redox mechanisms," December 2017, (Advisor).

Earle, M., (M.S.), "Iodine interactions with $AgNO_3$," May 2018 (Advisor).

Hoover, M., (Ph.D.), "Incorporation and surface calculations as probes for mineral alteration and growth," May 2019, (Advisor).

Johnston, I., (Ph.D.), "Coupling experimental measurements and computational models to probe the electronic double layer at mineral surfaces," May 2019, (Co-Advisor with Brian Powell).

TEACHING

Courses Taught

GEOL 2050, Mineralogy and Introductory Petrology, F12, F14, F15.
EE&S 4120, Nuclear Fuel Cycle and Waste Management, F15, F16.
EE&S 8120, Environmental Nuclear Engineering, F11, S13, S14, S16.
EE&S 8160, Technical Nuclear Forensics, S15.
EE&S 8830-012, Atomistic Modeling in Environmental Science, S13, S14.

UNIVERSITY AND PUBLIC SERVICE

Committees

Department: Member, EEES Geology Faculty Search Committee (2016 -)
Department: Member, EEES Nuclear Faculty Search Committee (2013 - 2014)
Department: Member, EEES Quality Assurance and Quality Control Committee (2013 -)
Department: Member, EEES Search Committee Toshiba Endowed Chair (2011 - 2012)
Department: Environmental Engineering and Science Undergraduate Recruiting (2011 -)
National: Member and series organizer, U.S. Department of Energy National Analytical Measurement Program (NAMP) Training and Education Committee (2013 -)
National: Member, Southeastern Universities Nuclear Fuel Management Advisory Board (2013)

MISCELLANEOUS

Carolina Nuclear Cluster member (2011 -)
Reviewer for Environmental Science and Technology, Journal of Nuclear Materials, Molecular Simulation, Journal of Solid State Chemistry, Industrial and Engineering Chemistry Research, Inorganic Chemistry
Proposal Reviewer for DOE-NEUP, DOE-BES-HEC.

Updated October 13, 2016.