MIXED WASTE

Analytical Chemistry & Instrumentation

Project: 54751

Title: High Fluence Neutron Source for Nondestructive Characterization of Nuclear Waste

PI: Dr. Mark M. Pickrell *Institution:* Los Alamos National Laboratory

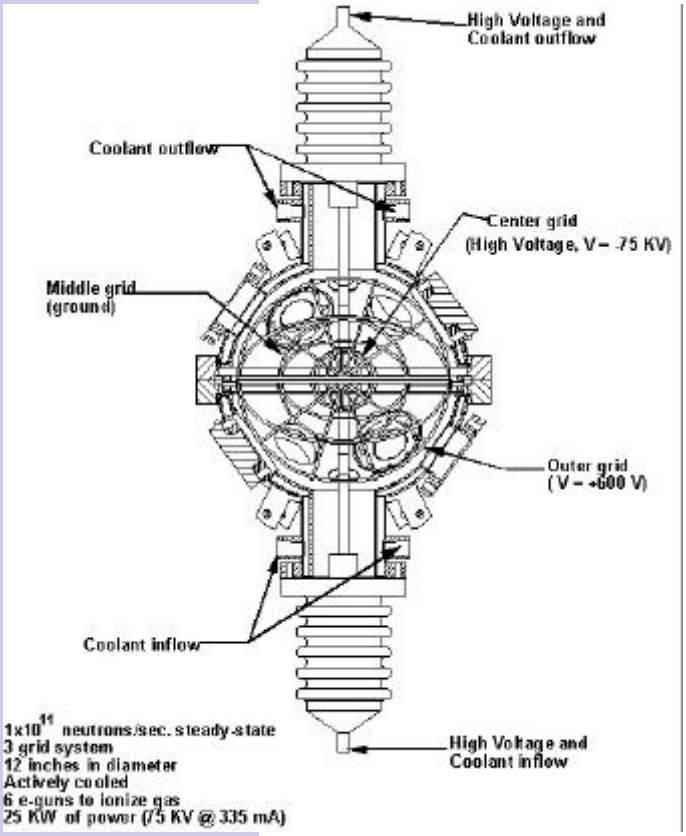
Publication Type: Journal

Barnes, D. C. & Nebel, R. A. (1998). Stable, thermal equilibrium. Large-amplitude, spherical plasma oscillations in electrostatic confinement devices. Physics of Plasmas, 5, 2498.

Nebel, R. A. & Barnes, D. C. (1998). The periodically oscillating plasma sphere. Fusion Tech. 38, 28.

Publication Type: Presentation

Nebel, R. A. & Barnes, D. C. (1997, Apr.). The periodically oscillating plasma sphere. Paper 1B-3 presented at the 1997 Sherwood Theory Meeting, Madison, WI.



Cutaway schematic of the Intense Neutron Source (INS). This source is to be used for assay applications, primarily for TRU waste. Its intensity should allow for real-time assay. [see Project #54751]

Nebel, R. A., Cole, A. J., & Umstadter, K. R. (1999, Oct.). The intense neutron source. Presentation at the 18th IEEE Symposium on Fusion Engineering, Albuquerque, NM.

Nebel, R. A., et. al. (1997). The Los Alamos intense neutron source. Winter ANS meeting, Albuquerque, NM.

Nebel, R. A., et. al. (1998). Innovative energy sources and advanced applications: The Los Alamos intense neutron source. Presentation at ECOMAP98, Kyoto, Japan.

Publication Type: Proceeding

Barnes, D. C., Nebel, R. A., Schauer, M. M., & Pickrell, M. M. (1997, May 19-21). Inertial electro-magnetostatic plasma neutron sources. Paper 7EO4, 1997 IEEE International Conference on Plasma Science, San Diego, CA. 319.

Nebel, R. A., et. al. (1997, Mar.). The Los Alamos intense neutron source. Proceedings of the 2nd Symposium on Current Trends in International Fusion Research: Review and Assessment. Washington, D. C.

Project: 55146

Title: Adsorption/Membrane Filtration as a Contaminant Concentration and Separation Process for Mixed Wastes and Tank Wastes

PI: Dr. Mark M. Benjamin *Institution:* University of Washington

Publication Type: Journal

Green-Pedersen, H. & Korshin, G. V. (1999). Separation of cesium from high ionic strength solutions using a cobalt hexacyanoferrate-modified graphite electrode. Environmental Science and Technology. 33(15), 2633-2637.

Project: 55171

Title: Development of Advanced In Situ Techniques for Chemistry Monitoring and Corrosion Mitigation in SCWO Environments

PI: Dr. Digby D. MacDonald *Institution:* Pennsylvania State University

Publication Type: Journal

Lvov, S. N., Zhou, X. Y., & Macdonald, D. D. (1999). Flow-through electrochemical cell for accurate pH measurements at temperatures up to 400°C. J. Electroanal. Chem. 463, 146-156.

Publication Type: Other

Lvov, S. N., Zhou, X. Y., Ulyanov, S. M., & Macdonald, S. N. (2000, in press). Potentiometric measurements of association constant and pH in high temperature HCI (aq) solutions. Tremaine, P. P. R., Hill, P. G., Irish, D. E., & Palakrishnan, P. V. (Eds.). Steam, Water, and Hydrothermal Systems: Physics and Chemistry. Meeting the Needs of Industry. Press Ottawa.

Zhou, X. Y., Lvov, S. N., & Ulyanov, S. M. (1998, Nov. 11). Safe Yttria-stabilized zirconia (YSZ) pH sensing electrode for high temperature aqueous systems. Invention Disclosure No. 98-1989.

Publication Type: Presentation

Lvov, S. N., et. al. (2000, Jun. 5). Reference systems for assessing viability and accuracy of pH sensors in high temperature subcritical and supercritical aqueous solutions. Chem. Geol. 167(1-2), 105-115.

Lvov, S. N., Zhou, X. Y., & Macdonald, S. N. (1998, May 3-8). Potentiometric pH measurements in supercritical aqueous solutions. The 193rd Meeting of the Electrochemical Society, Inc. Abstracts No. 1016. San Diego, CA.

Lvov, S. N., Zhou, X. Y., Wei, X. J., Ulyanov, S. M., & Macdonald, D. D. (1999, Aug. 22-26). Electrochemical corrosion studies in high temperature subcritical and supercritical aqueous environments. The 218th American Chemical Society Meeting, Abstract No. 129. New Orleans, LA.

Macdonald, D. D. (1997, May 11-14). Chemistry sensors for the universal solvents-supercritical aqueous solutions. Proceedings of the 4th International Symposium on Supercritical Fluids. Sendai, Japan. 861-864.

Macdonald, D. D. (1999, Nov. 10). The chemistry and electrochemistry of high subcritical and supercritical aqueous systems. Distinguished Lecturer Series, University of Toronto. Toronto, Canada.

Macdonald, D. D., Lvov, S. N., & Kriksunov, L. B. (1998, May 3-8). The chemical and electrochemical properties of supercritical aqueous solutions. The 193rd Meeting of the Electrochemical Society, Inc. Abstracts No. 1012. San Diego, CA.

Project: 59981

Title: Real-Time Broad Spectrum Characterization of Hazardous Waste by Membrane Introduction Mass Spectrometry

PI: Dr. Charles W. Wilkerson, Jr. *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Wilkerson Jr., C. W. (1999, Feb. 22-23). Workshop on harsh environment mass spectrometry. St. Petersburg, FL.

Wilkerson Jr., C. W. (1999, Feb. 28 - Mar. 4). WM99 - HLW, LLW, mixed wastes and environmental restoration - Working towards a cleaner environment. Tucson, AZ.

Wilkerson Jr., C. W. (1999, Mar. 7-12). Pittsburgh conference on analytical chemistry and applied spectroscopy. Orlando, FL.

Project: 60070

Title: The Development of Cavity Ringdown Spectroscopy as a Sensitive Continuous Emission Monitor for Metals

PI: Dr. George P. Miller *Institution:* Sensor Research and Developmenet Corporation

Publication Type: Journal

Miller, G. P. & Winstead, C. B. (1997). Inductively coupled plasma cavity ringdown spectroscopy. J. Anal. Atomic Spectro. 12, 907.

Winstead, C. B., Mazzotti, F. J., Mierzwa, J., & Miller, G. P. (1999, Jul.). Preliminary results for electrothermal atomization-cavity ringdown spectroscopy (ETA-CRDS). Anal. Commun. 36(7), 277-279.

Publication Type: Paper

Miller, G. P. (2000, in press). Determination of elemental mercury by cavity ringdown. Analyst.

Publication Type: Presentation

Miller, G. P. & Winstead, C. B. (1997, Jan. 12-17). ICP-cavity ringdown spectroscopy. Abstract O1-4, Winter Conference in Spectrochemistry. Gent, Belgium.

Miller, G. P. & Winstead, C. B. (1998, Oct. 12-15). ICP-cavity ringdown spectroscopy. Abstract 407, The 25th FACSS Conf. Austin, TX.

Miller, G. P. (2000, Sep. 25). Recent progress on analytical atomic cavity ringdown spectroscopy. FACSS conference, Nashville, TN.

Publication Type: Report

Miller, G. P. (2000, Oct.). Cavity ringdown laser absorption spectroscopy. In Meyers, R. A., Ed. Encyclopedia of Analytical Chemistry. Wiley & Sons, New York, NY.

Project: 73844 (Renewal of Project No. 60231)

Title: Miniature Chemical Sensor Combining Molecular Recognition with Evanescent-Wave Cavity Ring-Down Spectroscopy

PI: Dr. Andrew C. R. Pipino *Institution:* National Institute of Standards & Technology - Maryland

Publication Type: Journal

Pipino, A. C. R. (1998, Nov.). Evanescent wave cavity ring-down spectroscopy for ultra-sensitive chemical detection. SPIE 3535, 57. Boston, MA.

Pipino, A. C. R., et. al. (1997). Evanescent wave cavity ring-down spectroscopy with a total-internal-reflection minicavity. Rev. Sci. Instrum. 68, 2978.

Pipino, A.C.R., et. al. (1997). Evanescent wave cavity ring-down spectroscopy as a probe of surface processes. Chem. Phys. Lett. 280, 104.

Publication Type: Patent

Pipino, A. C. R. (1998, Nov. 10). Broad band intra-cavity total reflection chemical sensor. US #5,835,231.

Pipino, A. C. R. (1999, Aug. 24). Intra-cavity total reflection for high sensitivity measurement of optical properties. US #5,943,136.

Pipino, A. C. R. (1999, Nov. 16). Intra-cavity total reflection for high sensitivity measurement of optical properties. US #5,986,768.

Engineering Science

Project: 54973

Title: A Novel Energy-Efficient Plasma Chemical Process for the Destruction of Volatile Toxic Compounds

PI: Dr. Lal A. Pinnaduwage *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998). Enhanced negative ion formation by electron attachment to highly-excited molecules in a flowing plasma. J. Appl. Phys. 84, 3051.

Ding, W., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999). The role of high Rydberg states in enhanced o-formation in a pulsed O2 discharge. Plasma Sources Sci. Technol. 8, 384.

Ma, C. Y., McCorkle, D. L., Ding, W., & Pinnaduwage, L. A. (1999). A methodology for direct sampling and gas chromatographic/mass spectral analysis of volatile organic compounds emerging from a low pressure, flow-through reaction cell. J. Chromatography A. 844, 217.

Mabel, A. M., Lin, S. H., & Pinnaduwage, L. A. (1998). Potential energy surfaces of H2. Chem. Phys. Lett. 285, 114.

McCorkle, D. L., Ding, W. X., Ma, C. Y. & Pinnaduwage, L. A. (1999). Dissociation of benzene in a
pulsed glow discharge. J. Appl. Phys. 86, 3550.

McCorkle, D. L., Ding, W., Ma, C. Y., & Pinnaduwage, L. A. (1999). Exploratory studies on a plasma remediation process based on enhanced dissociative electron attachment to highly-excited molecules. J. Phys. D. 32, 46.

Pinnaduwage, L. A. & Datskos, P. G. (1997, Jun. 15). Electron attachment to excited states of silane: Implications for plasma processing discharges. J. Appl. Phys. 81(12), 7715-7727.

Pinnaduwage, L. A., et. al. (1999). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. J.Appl. Phys. 85, 7064.

Pinnaduwage, L. A., McCorkle, D. L., & Ding, W. (1997). Enhanced electron attachment to highly excited molecules using a plasma mixing scheme. Appl. Phys. Lett. 71, 3634.

Pinnaduwage, L. A., Tav, C., McCorkle, D. L., & Ding, W. (1999). Temperature dependence of electron attachment to methylene chloride. J. Chem. Phys. 110, 9011.

Publication Type: Patent

Pinnaduwage, L. A. (1999, Apr. 20). Plasma mixing glow discharge device for analytical applications. US Patent #5,896,196.

Publication Type: Presentation

Ding, W. X., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Decomposition of volatile organic compounds in a positive column glow discharge plasma. Presentation at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W. X., Pinnaduwage, L. A., Tav, C., & McCorkle, D. L. (1999, Mar. 20-26). O- formation by electron attachment to high Rydberg states. Presented at the 1999 Centennial Meeting of the American Physical Society. Atlanta, GA.

Ding, W., Ma, C. Y., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Decomposition of volatile organic compounds in a positive column glow discharge plasma. Presented at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W., McCorkle, D. L., & Pinnaduwage, L. A. (1998, Jun. 1-4). Enhanced radical formation by electron attachment to highly-excited states of molecules in plasmas. Presented at the 25th IEEE International Conference on Plasma Science. Raleigh, NC.

Ding, W., McCorkle, D. L., Ma, C. Y., & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociation of benzene in a pulsed glow discharge. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Ma, C. Y., McCorkle, D. L., Ding, W., & Pinnaduwage, L. A. (1998, May 31 - Jun. 4). Methodology for direct sampling of volatile organic compounds emerging from a low-pressure, flow-through reaction cell for subsequent GC-GC/MS analysis. Presented at the 46th ASMS Conference on Mass Spectrometry and Allied Topics. Orlando, FL.

McCorkle, D. L. & Pinnaduwage, L. A. (1997, Oct. 6-9). Destruction of CH2Cl2 using a glow discharge scheme. 50th Annual Gaseous Electronics Conference. Madison, WI.

Pinnaduwage, L. A. (1997, Jun. 29 - Jul. 2). Implications of electron attachment to highly-excited states in pulsed power discharges. 11th IEEE Pulsed Power Conference. Baltimore, MA.

Pinnaduwage, L. A. (1999, Sep. 22). Novel energy-efficient plasma chemical process for the destruction of volatile toxic compounds. DOE Environmental Management Science Program Workshop. Oak Ridge, TN.

Pinnaduwage, L. A., Datskos, P. G., Ding, W. X., & McCorkle, D. L. (1998, Jun. 27 - Jul. 3). Enhanced electron attachment to highly-excited states of molecules: Implications for plasma processing discharges. Presentation at the 1998 International Congress on Plasma Physics. Prague, Czech Republic.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1999, Mar. 20-26). Enhanced electron attachment to Rydberg states in molecular hydrogen volume discharges. Presented at the 1999 Centennial Meeting of the American Physical Society. Atlanta, GA.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1998, Jun. 27 - Jul. 3). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Presented at the 1998 International Congress on Plasma Physics. Prague, Czech Republic.

Pinnaduwage, L. A., Ding, W. X., McCorkle, D. L., & Ma, C. Y. (1999, Jun. 27-30). Implications of electron attachment to highly-excited states of molecules and its applications in pulsed plasmas. 12th IEEE Pulsed Power Conference. Monterrey, CA.

Pinnaduwage, L. A., Ding, W., & McCorkle, D. L. (1999, Oct. 5-8). Negative ion formation in pulsed plasmas. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Pinnaduwage, L. A., Ma, C. Y., McCorkle, D. L., & Ding, W. (1998, Jul. 27-30). A novel energy-efficient plasma chemical process for the destruction of volatile toxic compounds. Presented at the Environmental Management Science Program Workshop. Chicago, IL.

Tav, C. & Pinnaduwage, L. A. (1999, Oct. 5-8). Dissociative electron attachment to laser-excited benzene. 52nd Annual Gaseous Electronics Conference. Norfolk, VA.

Publication Type: Proceeding

Pinnaduwage, L. A. (1997). Implications of electron attachment to highly-excited states in pulsed power discharges. Cooperstein, G. & Vitkovitsky, I. (Eds.). Digest of Technical Papers of the 11th IEEE Pulsed Power Conference. IEEE Publishing Services. New York, NY. 1048-1053.

Pinnaduwage, L. A., Datskos, P. G., Ding, W. X., & McCorkle, D. L. (1999). Enhanced electron attachment to highly-excited states of molecules: Implications for plasma processing discharges. Pavlo, P. (Ed.). Proceedings of the 1998 International Congress on Plasma Physics. 125-128.

Pinnaduwage, L. A., Ding, W. X., & McCorkle, D. L. (1999). Enhanced electron attachment to superexcited Rydberg states of molecular hydrogen using a plasma mixing scheme. Pavlo, P. (Ed.). Proceedings of the 1998 International Congress on Plasma Physics. 129-132.

Pinnaduwage, L. A., Ding, W. X., McCorkle, D. L., & Ma, C. Y. (1999). Enhanced electron attachment to highly-excited molecules and its applications in pulsed plasmas. Stallings, C. & Kirbie, H. (Eds.). Digest of Technical Papers of the 12th IEEE Pulsed Power Conference. IEEE Publishing Services. New York, NY. 1322-1325

Publication Type: Theses/Dissertations

Tav, C. (2000). Enhanced electron attachment to vibrationally and electrically excited molecules. Ph. D. dissertation.

Project: 60155

Title: Measurements and Models for Hazardous Chemical and Mixed Wastes
PI: Dr. Cynthia Holcomb *Institution:* National Institute of Standards & Technology - Boulder

Publication Type: Journal

Mathias, P. M., Naheiri, T., & Oh, E. M. (1989). A density correction for the Peng-Robinson equation of state. Fluid Phase Equilibria. 47, 77-87.

Inorganic Chemistry

Project: 54506

Title: Acid-Base Behavior in Hydrothermal Processing of Wastes
PI: Dr. Keith P. Johnston *Institution:* University of Texas at Austin

Publication Type: Journal

Chlistunoff, J. B., Ziegler, K. J., Lasdon, L., & Johnston, K. P. (1999). Nitric/nitrous acid equilibria in supercritical water. Journal of Phys. Chem. B. 103, 1678-1688.

Johnston, K. P. & Chlistunoff, J. B. (1998). Neutralization of acids and bases in subcritical and supercritical water: Acetic acid and HCl. J. Supercrit. Fluid. 12, 155-64.

Ziegler, K. J., Lasdon, L., Chlistunoff, J., & Johnston, K. P. (1999). Optimization models for determining nitric acid equilibria in supercritical water. Comput. Chem. 23(5), 421-434.

Publication Type: Report

Johnston, K. P. & Rossky, P. J. (1999, in press). Solution chemistry in supercritical water: spectroscopy and simulation. E. Kiran (Ed.), NATO Adv. Study Institute on Supercritical Fluids.

Project: 55276

Title: Fundamental Chemistry and Thermodynamics of Hydrothermal Oxidation Processes

PI: Dr. John M. Simonson *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Blencoe, J. G., Anovitz, L. M., & Seitz, J. C. (1998, in press). A new method for modeling the thermodynamic mixing properties of high-temperature H2 O-CO2 fluids. Eos. 79.

Blencoe, J. G., Seitz, J. C., & Anovitz, L. M., (1999, in press). The CO2 -H2 O System. II. Calculated Thermodynamic Mixing Properties for 400°C, 0-400 MPa. Geochim. Cosmochim. Acta. 63.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1999, Jan. 8). Solvation in high-temperature electrolyte solutions. II. Some formal results. J. Chem. Phys. 110(2), 1075-1086.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1999, Jan. 8). Solvation in high-temperature electrolyte solutions. I. Hydration shell behavior from molecular simulation. J. Chem. Phys. 110(2), 1064-1074.

Chialvo, A. A., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (1998). Thermodynamics and kinetics of ion speciation in supercritical aqueous solutions: A molecular-based study. Fluid Phase Equilibria. 150-151, 107-115.

Chialvo, A. A., Kusalik, P.G., Cummings, P. T., Simonson, J. M., & Mesmer, R. E. (2000, Apr. 17.). Molecular approach to high temperature solvation. Formal, integral equation, and experimental results. J. Phys-Condens. Mat. 12(15), 3585-3593.

Dai, S., Burleigh, M., Simonson, J. M., Mesmer, R. E., & Xue, Z. -L. (1998). Application of chemometric methods in UV-Vis absorption spectroscopic studies of uranyl ion dimerization reaction in aqueous solutions. Radiochimica Acta. 81, 195-199.

Moore, R. C., Mesmer, R. E., & Simonson, J. M. (1997). The solubility of potassium carbonate in water between 384 and 529 K measured using the synthetic method. J. Chem. Eng. Data. 42, 1078-1081.

Seitz, J. C. & Blencoe, J. G. (1999, in press). The CO2 -H2 O System. I. Experimental Determination of Volumetric Properties at 400°C, 10-100 MPa. Geochim. Cosmochim. Acta. 63.

Publication Type: Presentation

Blencoe, J. G., Anovitz, L. M. & Seitz, J. C. (1998). A Helmholz free energy model for supercritical H2 O-CO2 mixtures. Geol. Soc. Amer. Abs. with Prog. 30, A-319.

Blencoe, J. G., Anovitz, L. M., Seitz, J. C. (1997). Serious shortcomings of semi-empirical equations of state for high-temperature aqueous C-O-H-N fluids. Geol. Soc. Amer. Abs. with Prog. 29, A-210.

Seitz, J. C. & Blencoe, J. G. (1997). Experimentally determined volumetric properties and solvus relations for H2 O-CO2 -N2 mixtures at 300°C and pressures < 1000 bars. Geol. Soc. Amer. Abs. with Prog. 29, A-209.

Singh, J., Blencoe, J. G., & Seitz, J. C., (1998). Experimentally determined excess molar volumes for H2 O-N2 fluids at 300°C, 75-1000 bars. Geol. Soc. Amer. Abs. with Prog. 30, A-319.

Project: 59934

Title: Hazardous Gas Production by Alpha Particles in Solid Organic Transuranic Waste Matrices

PI: Dr. Jay A. LaVerne *Institution:* University of Notre Dame

Publication Type: Journal

Chang, Z. & La Verne, J. A. (2000). Hydrogen production in the heavy ion radiolysis of polymers: I. Polyethylene, polypropylene, poly(methyl methacrylate) and polystyrene. J. Phys. Chem. B. 104, 10557-10562.

Chang, Z. & LaVerne, J. A. (1999). Molecular hydrogen production in the radiolysis of high density polyethylene. J. Phys. Chem. B. 103, 8267-8271.

Chang, Z. & LaVerne, J. A. (1999). The yield of hydrogen gas in the gamma-ray and heavy-ion radiolysis of high density polyethylene. J. Phys. Chem. B. 103, 8267-8271.

Chang, Z. & LaVerne, J. A. (2000). Hydrogen production in the heavy ion radiolysis of polyethylene, polypropylene, poly(methyl methacrylate) and polystyrene. J. Poly. Sci. A. Poly. Chem. 38, 1656-1661.

Chang, Z. & LaVerne, J. A. (2000). Hydrogen production in y-ray and helium ion radiolysis of polyethylene, polypropylene, poly(methyl-methacrylate) and polystyrene. J. Poly. Sci. 38, 000-000.

Chang, Z. & LaVerne, J. A. (2001, in press). The gases produced in the gamma and heavy-ion radiolysis of poly(methyl methacrylate). Radiat. Phys. Chem.

LaVerne, J. A., Chang, Z., & Araos, M. S. (2001, in press). Heavy ion radiolysis of organic materials. Radiat. Phys. Chem.

Publication Type: Poster

Chang, Z. (1999, Aug. 21-25). Production of hydrogen gas in the heavy-ion radiolysis of high-density polyethylene. 218th American Chemical Society National Meeting. New Orleans, LA.

LaVerne, J. A. & Chang, Z. (1999, Aug. 21-25). Hydrogen production in the radiolysis of polymers. 218th American Chemical Society National Meeting. New Orleans, LA.

LaVerne, J. A. & Chang, Z. (2000, Jun. 25-30). Production of hydrogen in the heavy ion radiolysis of polymers. Gordon Conference on Radiation Chemistry. Plymouth, NH.

Publication Type: Presentation

LaVerne, J. A. (2000, Mar. 14). Heavy ion radiolysis of organic materials. Invited presentation at the International Symposium on Prospects for Application of Radiation Towards the 21st Century. Waseda University. Waseda, Japan.

Materials Science

Project: 55387

Title: Photooxidation of Organic Waste Using Semiconductor Nanoclusters

PI: Dr. Jess P. Wilcoxon *Institution:* Sandia National Laboratories - Albuquerque

Publication Type: Journal

Parsapour, F., Kelley, D. F., Craft, S., & Wilcoxon, J. P. (1996). Electron transfer dynamics in MoS2 nanoclusters: Normal and inverted behavior. J. Chem. Phys. 104, 1.

Thurston, T. R. & Wilcoxon, J. P. (1998). Photo-oxidation of organic chemicals catalyzed by nanoscale MoS2. J. Phys. Chem. 103, 11.

Wilcoxon, J. P., Newcomer, P., & Samara, G. A. (1997). Synthesis and optical properties of MoS2 and isomorphous nanoclusters in the quantum confinement regime. J. Appl. Phys. 81, 7934.

Publication Type: Patent

Wilcoxon, J. P. (1999, Jan.). Visible light photooxidation of toxic organic chemicals using nanoscale MoS2. DOE Technical Advance Patent Application filed Jan. 1999.

Publication Type: Proceeding

Wilcoxon, J. P. & Thurston, T. R. (1998). Photocatalysis using nanosize semiconductors. Proceedings of Symposium FF, Fall MRS Meeting. Boston, MA.

Wilcoxon, J. P., Parsapour, R., & Kelley, D. F. (1997, May 4-9). Studies of photoredox reactions on nanosize semiconductors. 4th International Conference on Quantum Confinement: Nanoscale Materials, Devices, and Systems. 119th Meeting of the Electrochemical Society. Montreal, Quebec, Canada.

Microbial Science

Project: 73833 (Renewal of Project No. 60150)

Title: Genetic Engineering of a Radiation-resistant Bacterium for Biodegradation of Mixed Wastes

PI: Dr. Mary E. Lidstrom *Institution:* University of Washington

Publication Type: Poster

Meima, R., Rothfuss, H., Gewin, L., & Lidstrom, M. E. (1998, Jul. 27-30). Genetic engineering of a radiation-resistant bacterium for biodegradation of mixed wastes. Poster presentation at the DOE Environmental Management Science Program Workshop. Chicago, IL.

Separations Chemistry

Project: 54571

Title: Removal of Heavy Metals and Organic Contaminants from Aqueous Streams by Novel Filtration Methods

PI: Dr. Nelly M. Rodriguez

Institution: Northeastern University

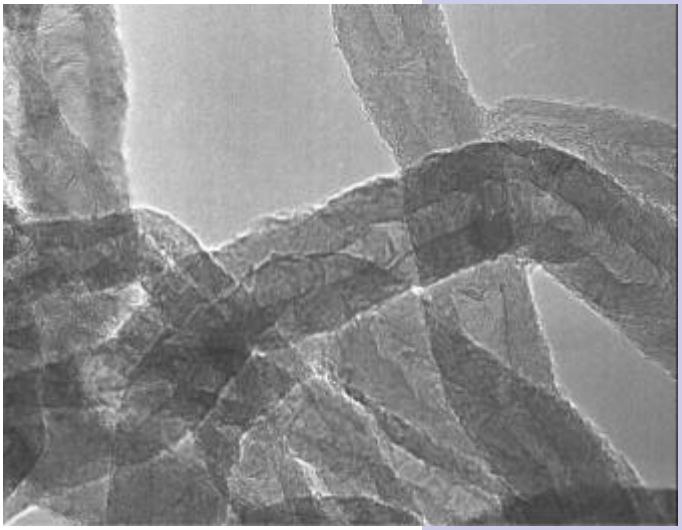
Publication Type: Journal

Anderson, P. E. & Rodriguez, N. M. (1999). Synthesis of graphite nanofibers from the decomposition of CO/H2 over silica supported iron-nickel particles. J. Mat. Res. 14, 2912.

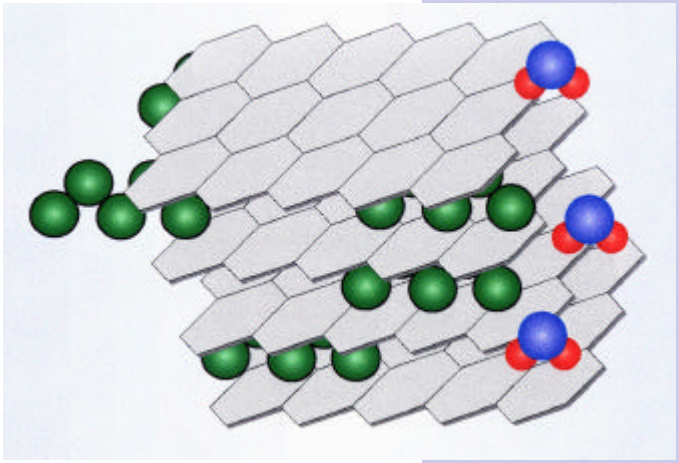
Anderson, P. E. & Rodriguez, N. M. (1999, Jul.). Growth of graphite nanofibers from the decomposition of CO/H2 over silica supported iron-nickel particles. J. Mater. Res. 14(7), 2912-2921.

Anderson, P. E. & Rodriguez, N. M. (2000). Synthesis of graphite nanofibers over transition metal catalysts supported on various substrates. Chem. Of Mat. 12, 823.

Anderson, P. E. & Rodriguez, N. M. (2000, in press). Effect of the support on the synthesis of carbon nanofibers. Mat. Res. Soc. Symp. Proc.



Transmission electron micrograph (TEM) of carbon nanofibers. [see Project #54571]



Organic impurity molecules being trapped between the graphene layers of a carbon nanofiber. Water molecules are preferentially absorbed at the edge sites of the structure. [see Project #54571]

Anderson, P. E., Engel, E., Crowe, A., Park, C., & Rodriguez, N. M. (2000, Mar.). Influence of the support on the structural characteristics of carbon nanofibers produced from the metal-catalyzed decomposition of ethylene. Chem. Mater. 12(3), 823-830.

Park, C., Anderson, P. E., & Chambers, A. (1999, Dec. 2). Further studies of the interaction of hydrogen with graphite nanofibers. J. Phys. Chem. B. 103(48), 10572-10581.

Park, C., Engel, E., Crowe, A., Gilbert, T. R., & Rodriguez, N. M. (2000, in press). Removal of organic molecules from aqueous solutions using graphite nanofibers. Langmuir.

Publication Type: Proceeding

Anderson, P. E., Engel, E., Crowe, A., Park, C., & Rodriguez, N. M. (2000). Carbon nanofibers for environmental applications. Proceedings of the WM2000 Conference. Tucson, AZ.

Project: 54770

Title: New Anion-Exchange Resins for Improved Separations of Nuclear Materials
PI: Dr. Mary E. Barr *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Marsh, S. F., Jarvinen, G. D., & Bartsch, R. A. (1997). New bifunctional anion-exchange resins for nuclear waste treatment. Reactive Polymers. 35, 75-80.

Marsh, S. F., Jarvinen, G. D., Bartsch, R. A., Nam, J., & Barr, M. E. (1998). New bifunctional anion-exchange resins for nuclear waste treatment-II. J. Radioanal. Nucl. Chem. 235, 37-40.

Publication Type: Presentation

Barr, M. E., Jarvinen, G. D., Marsh, S. F., & Bartsch, R. A. (1997, Apr. 13). Development of anion-exchange resins for separations of actinides. Abstracts of Papers of the American Chemical Society. 213(pt.2), 73-IEC.

Barr, M. E., Jarvinen, G. D., Moody, E. W., & Vaughn, R. B. (1998, Aug. 23). Sorption of Pu(IV) by soluble anion-exchange polymers. Abstracts of Papers of the American Chemical Society. 216(pt.2), 88-NUCL, & 216(pt.1), 5-TECH.

Barr, M. E., Jarvinen, G. D., Schulte, L. D., Stark, P. C., & Chamberlin, R. M. (1999, Mar. 21). Americium separations from complex mixtures using anion exchange. Abstracts of Papers of the American Chemical Society. 217, 019-IEC.

Bartsch, R. A., et. al. (1999, Mar. 21). Sorption of Pu(IV) from nitric acid by bifunctional anion-exchange resins. Abstracts of Papers of the American Chemical Society. 217, 125-IEC.

Marsh, S. F., Jarvinen, G. D., Bartsch, R. A., Nam, J., & Barr, M. E. (1997, Apr.). New bifunctional anion-exchange resins for nuclear waste treatment. Marc IV conference on Radioanalytical Chemistry, Kona, HI.

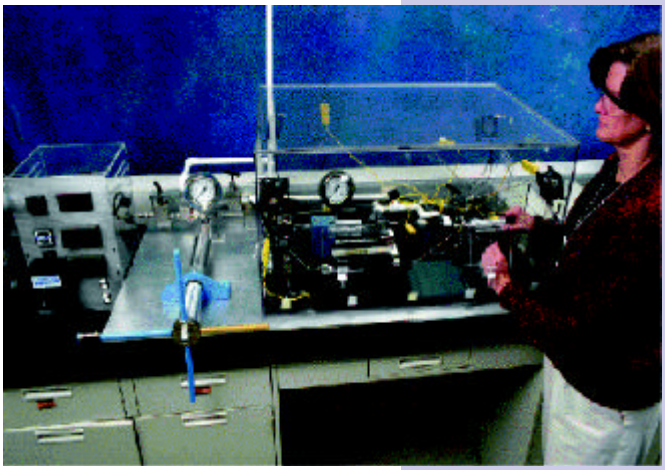
Moody, E. W., Barr, M. E., & Jarvinen, G. D. (1999). QSAR of distribution coefficients for actinide hexanitrato complexes. Abstracts of Papers of the American Chemical Society. 217(pt.2), 170-NUCL.

Project: 54847

Title: Photocatalytic and Chemical Oxidation of Organic Compounds in Supercritical Carbon Dioxide
PI: Dr. Daniel M. Blake
Institution: National Renewable Energy Laboratory

Publication Type: Journal

Jacoby, W. A., et al. (1996). Heterogeneous photocatalysis for control of volatile organic compounds in indoor air. J. Air Waste Manage. Assoc. 46(9), 891-898.



A National Renewable Energy Laboratory project uses an experimental system to study photocatalytic oxidation of organic substances in supercritical carbon dioxide. Organic compounds are monitored by an online gas chromatograph or by UV-visible spectroscopy. [see Project #54847]

Project: 54942

Title: Spectroscopy, Modeling and Computation of Metal Chelate Solubility in Supercritical CO_2
PI: Dr. Joan F. Brennecke
Institution: University of Notre Dame

Publication Type: Journal

Brennecke, J. F. & Chateauneuf, J. E. (1999). Homogeneous organic reactions as mechanistic probes in supercritical fluids. Chemical Reviews. 99(2), 433-452.

Hua, J. Z., Brennecke, J. F., & Stadtherr, M. A. (1998). Enhanced interval analysis for phase stability: Cubic equation of state models. Ind. Eng. Chem. Res. 37, 1519-1527.

Hua, J. Z., Brennecke, J. F., & Stadtherr, M. A. (1998). Reliable computation of phase stability using interval analysis: Cubic equation of state models. Computers and Chemical Engineering. 22, 1207-1214.

Hua, J. Z., Maier, R. W., Tessier, S. R., Brennecke, J. F., & Stadtherr, M. A. (1999). Interval analysis for thermodynamic calculations in process design: A novel and completely reliable approach. Fluid Phase Equilibria, 158-160, 607-615.

Maier, R. W., Brennecke, J. F., & Stadtherr, M. A. (1998). Reliable computation of homogeneous azeotropes. AIChE J. 44, 1745-1755.

Maier, R. W., Brennecke, J. F., & Stadtherr, M. A. (1999, in press). Computing homogeneous azeotropes using interval analysis. Chem. Eng. & Tech.

Stadtherr, M. A. (1999). High performance computing: Are we just getting wrong answers faster? AIChE CAST Communications. 22(1), 6-14.

Tessier, S. R., Brennecke, J. F., & Stadtherr, M. A. (1999, in press). Reliable phase stability analysis for excess Gibbs energy models. Chemical Engineering Science.

Xu, G., Scurto, A. M., Castier, M., Brennecke, J. F., & Stadtherr, M. A. (1999, in press). Reliable computation of high pressure solid-fluid equilibrium. Ind. Eng. Chem. Res.

Publication Type: Poster

Chateauneuf, J. E. (1999, Aug. 23). The use of reaction intermediates to probe supercritical fluid solvent effects. American Chemical Society 218th National Meeting. New Orleans, LA.

Chateauneuf, J. E., Zhang, J., Brink, J., Slominis, M., & Perkovic, M. (1999, Mar. 24). Investigation of free radical ion reactivity with supercritical carbon dioxide. Physical Chemistry Division, Free Radicals in the Condensed Phase Symposium. American Chemical Society 217th National Meeting. Anaheim, CA.

Chateauneuf, J. E., Zhang, J., Brink, J., Slominis, M., & Perkovic, M. (1999, Mar. 22). Investigation of free radical and radical ion reactivity with supercritical carbon dioxide. Poster presentation at the Sci-Mix Division of the American Chemical Society 217th National Meeting, Anaheim, CA.

Hua, J. Z., Maier, R. W., Tessier, S. R., Brennecke, J. F., & Stadtherr, M. A. (1998, Apr. 26 - May 1). Interval analysis for thermodynamic calculations in process design: A novel and completely reliable approach. Eighth International Conference on Properties and Phase Equilibria for Product and Process Design. Noordwijkerhout, The Netherlands.

Publication Type: Presentation

Brennecke, J. F. & Stadtherr, M. A. (1999, May 27). Reliable computation of phase behavior using interval analysis. Escola de Quimica, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil.

Brennecke, J. F. (1997, Nov. 6). Supercritical fluids for environmental applications: A chemical engineering perspective. Department of Chemistry, Western Michigan University, Kalamazoo, MI.

Brennecke, J. F. (1998, Apr. 13-16). Dense phase fluids: Phase behavior. Department of Energy/Environmental Protection Agency Dense Phase Fluids and Alternative Reaction Media Workshop, Santa Fe, NM.

Brennecke, J. F. (1998, Apr. 16). Thermodynamic and kinetic studies in supercritical fluids. Department of Chemistry, Loyola University of Chicago, Chicago, IL.

Brennecke, J. F. (1998, Oct. 1). Using spectroscopy to understand metal chelates in supercritical CO2. Department of Chemical Engineering, University of Massachussettes, Amherst, MA.

Brennecke, J. F. (1998, Sep. 9). Understanding metal chelates in supercritical CO2. Department of Chemical Engineering, University of Texas at Austin, Austin, TX.

Brennecke, J. F. (1999, Apr. 10-13). Spectroscopy to measure solvation, kinetics, and equilibrium in supercritical fluids. 6th Meeting on Supercritical Fluids: Chemistry and Materials, Nottingham, U. K.

Brennecke, J. F. (1999, Apr. 30). Polution prevention with supercritical CO2. Department of Civil Engineering, Northwestern University, Evanston, IL.

Brennecke, J. F. (1999, Jun. 1). Spectroscopic measurements of local compositions. PLAPIQUI, Universidad Nacional del Sur, Bahia Blanca, Argentina.

Brennecke, J. F. (1999, Jun. 4). Application of supercritical chemical engineering processes in environmental protection and remediation. PLAPIQUI, Universidad Nacional del Sur, Bahia Blanca, Argentina.

Brennecke, J. F. (1999, May 25). Environmental applications of supercritical fluids. Escola de Quimica, Universidade Federal do Rio de Janeiro, Rio de Janeiro, Brazil.

Brennecke, J. F., Stadtherr, M. A., & Chateauneuf, J. E. (1998, Jul. 27-30). Spectroscopy, modeling, and computation of metal chelate solubility in supercritical CO2. Department of Energy EMSP Scientific Workshop, Rosemont, IL.

Chateauneuf, J. E. (1998, Mar. 1). The use of reaction intermediates to investigate supercritical fluid solvent effects: The development of supercritical fluids as environmentally benign reaction media. Department of Chemistry, Central Michigan University, Mt. Pleasant, MI.

Chateauneuf, J. E. (1999, Aug. 22-26). The use of reaction intermediates to probe supercritical fluid solvent effects. Symposium on Chemistry of Reactive Intermediates and Modeling in Hydrocarbon Conversion. American Chemical Society 218th National Meeting. New Orleans, LA.

Chateauneuf, J. E. (1999, Jul. 11-16). Free radical reactions in supercritical fluids. Gordon Research Conference on Free Radical Reactions, Holderness School, Plymouth, NH.

Chateauneuf, J. E. (1999, Jun. 30). Reactions in supercritical fluids: The development of supercritical fluids as environmentally benign reaction media. Department of Chemistry, Argonne National Laboratory, Argonne, IL.

Chateauneuf, J. E. (1999, Mar. 3). The development of supercritical fluids as environmentally benign reaction media: The influence of SCF solvation on chemical reactivity. Department of Chemistry and the Center for Photochemical Sciences, Bowling Green State University, Bowling Green, OH.

Chateauneuf, J. E. (1999, May 19). Reactions in supercritical fluids: The development of supercritical fluids as environmentally benign reaction media. Department of Chemistry, Andrews University, Berrien Springs, MI.

Hua, J. Z., Brennecke, J. F., & Stadtherr, M. A. (1997, Nov. 16-21). Combined local and global approach to reliable computation of phase eqilibria. Annual AIChE Meeting. Los Angeles, CA.

Maier, R. W., Brennecke, J. F., & Stadtherr, M. A. (1998, Nov. 15-20). Computation of reactive azeotropes using interval analysis. Annual AIChE Meeting. Miami, FL.

Maier, R. W., Brennecke, J. F., & Stadtherr, M. A. (1999, Oct. 31-Nov. 5). A new approach for reliably computing all azeotropes of multicomponent mixtures. Annual AIChE Meeting. Dallas, TX.

Maier, R. W., Brennecke, J. F., & Stadtherr, M. A. (1997, Nov. 16-21). A new approach for reliable computation of homogenous azeotropes in multicomponent mixtures. AIChE Annual Meeting. Los Angeles, CA.

Maier, R. W., Stadtherr, M. A., & Brennecke, J. F. (1998, May 18-19). Reliable computation of homogenous azeotropes. 1998 Midwest Thermodynamics and Statistical Mechanics Conference. Notre Dame, IN.

Roggeman, E. J., Scurto, A. M., Brennecke, J. F., & Chateauneuf, J. E. (1998, May 18-19). Spectroscopic measurements of preferential solvation and novel solubility measurements of metal chelate complexes in pure and modified supercritical CO2. 1998 Midwest Thermodynamics and Statistical Mechanics Conference. Notre Dame, IN.

Roggeman, E. J., Scurto, A. M., Chateauneuf, J. E., & Brennecke, J. F. (1998, Nov. 15-20). Cosolvent effects to enhance metal extraction with supercritical CO2. Annual AIChE Meeting. Miami, FL.

Roggeman, E. J., Scurto, A. M., Stadherr, M. A., & Brennecke, J. F. (1998, Jul. 12-16). Spectroscopy, measurement, and modeling of metal chelate solubility in supercritical CO2. 8th International Symposium on Supercritical Fluid Chromatography and Extraction, St. Louis, MO.

Stadtherr, M. A. (1998, Feb. 24). Reliable process modeling using interval analysis. Department of Chemical Engineering Seminar, Carnegie-Mellon University, Pittsburgh, PA.

Stadtherr, M. A. (1998, Nov. 15-20). High performance computing: Are we just getting wrong answers faster? Computing and Systems Technology Division Awards Dinner, AIChE Annual Meeting, Miami Beach, FL.

Stadtherr, M. A. (2000, Feb. 6-11). Recent advances in reliable nonlinear equation solving. Aspen World 2000. Orlando, FL.

Stadtherr, M. A. (2000, Mar. 29). Reliable process modeling using interval analysis. Department of Chemical Engineering Seminar. University of Kansas, Lawrence, KS.

Stadtherr, M. A., Hua, J. Z., & Brennecke, J. F. (1997, Oct. 26-29). Phase stability analysis for equation of state models. Institute for Operations Research and the Management Sciences, National Meeting, Dallas, TX.

Stadtherr, M. A., Maier, R. W., & Gau, C.-Y. (1999, Oct. 31-Nov. 5). New interval methodologies for reliable process modeling. AIChE Annual Meeting. Dallas, TX.

Stadtherr, M. A., Maier, R. W., Stradi, B. A., Xu, G., & Brennecke, J. F. (1998, Nov. 15-20). Reliable computation of high pressure phase behavior. Annual AIChE Meeting. Miami, FL.

Stadtherr, M. A., Xu, G., Stradi, B., Maier, R. W., & Brennecke, J. F. (1999, May 12-15). Reliable computation of phase behavior using interval methods. SIAM Annual Meeting, Atlanta, GA.

Xu, G., Brennecke, J. F., & Stadtherr, M. A. (1999, Oct. 31-Nov. 5). Reliable computation of solid-supercritical fluid equilibria using interval analysis. Annual AIChE Meeting. Dallas, TX.

Xu, G., Brennecke, J. F., & Stadtherr, M. A. (1999, May 17-18). Reliable computation of solid-fluid equilibria using interval analysis. Midwest Thermodynamics and Statistical Mechanics Conference. Detroit, MI.

Xu, G., Scurto, A. M., Castier, M., Stadtherr, M. A., & Brennecke, J. F. (2000, Apr. 8-12). Reliable computation of high pressure solid-fluid equilibrium. 5th International Symposium on Supercritical Fluids. Atlanta, GA.

Xu, G., Scurto, A. M., Castier, M., Stadtherr, M. A., & Brennecke, J. F. (2000, Sep. 24-27). Reliable computation of high pressure solid-fluid equilibrium. Presented in conjunction with Western Michigan University (subcontract) at COBEQ 2000. Aguas de Sao Pedro, Brazil.

Zhang, J., Roggeman, E. J., Chateauneuf, J. E., & Brennecke, J. F. (1997, Nov. 16-21). Cosolvent effects on metal chelates in supercritical CO2. Annual AIChE Meeting. Los Angeles, CA.

Publication Type: Proceeding

Kremer, M. J., et. al. (1999, Apr. 10-13). Spectroscopy to measure solvation, kinetics, and equilibrium in supercritical fluids. Proceedings of the 6th Meeting on Supercritical Fluids: Chemistry and Materials. Nottingham, U. K.

Roggeman, E. J., Scurto, A. M., Stadtherr, M. A., & Brennecke, J. F. (1998, Jul. 12-16). Spectroscopy, measurement and modeling of metal chelate solubility in supercritical CO2. Proceedings of the 8th International Symposium on Supercritical Fluid Chromatography and Extraction, St. Louis, MO.

Publication Type: Theses/Dissertations

Jin, H. (1999, Jul.). Spectroscopic investigations of carbocation reactivity in supercritical carbon dioxide. M. S. Thesis.

Zhang, J. (expected 2000). M. S. Thesis.

Project: 55103

Title: Utilization of Kinetic Isotope Effects for the Concentration of Tritium
PI: Dr. Gilbert M. Brown *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Huynh, M. H. V., El-Samonody, E-S., Meyer, T. J., & White, P. S. (1999, Aug. 23). The effect of stepwise oxidation on molecular structure in osmium hydrazido complexes. Inorg. Chem. 38(17), 3760+.

Huynh, M. H. V., et. al. (1999). Oxo-like reactivity of high oxidation state osmium hydrazido complexes. Journal of American Chemical Society. 121, 1403-1404.

Huynh, M. H. V., White, P. S., & Meyer, T. J. (1999, May 12). Proton-coupled electron transfer from nitrogen: A N-H/N-D kinetic isotope effect of 41.4. J. Am. Chem. Soc. 121(18), 4530-4531.

Lebeau, E. L. & Meyer, T.J. (1999). Oxidation of benzyl alcohol by a dioxo complex of Ru(VI). Inorganic Chemistry. 38, 2174-2181.

Trammell, S. A., et. al. (1998). Mechanisms of surface electron transfer: Proton-coupled electron transfer. Journal of American Chemical Society. 120, 13248-13249.

Publication Type: Proceeding

Barton, J. W., Klasson, K. T., & Davison, B. H. (1997). Extended operation and control of biomass overgrowth in biofiliters designed for VOC removal. Proceedings of the 90th Annual Meeting & Exhibition of Air and Waste Management Association. Toronto, Ontario, Canada.

Project: 60096

Title: Rational Synthesis of Imprinted Organofunctional Sol-Gel Materials for Toxic Metal Separation

PI: Dr. Ziling Benjamin Xue *Institution:* University of Tennessee at Knoxville

Publication Type: Journal

Dai, S., et. al. (1999). Imprint coating: Novel synthesis of selective functionalized ordered mesoporous sorbents. Angew. Chem. Int. Ed. 38, 1235-1239.

Dai, S., et. al. (1999, Oct. 1). A new methodology to functionalize surfaces of ordered mesoporous materials based on ion exchange reactions. Adv. Mater. 11(14), 1226-1230.

Shin, Y. S., Burleigh, M. C., Dai, S., Barnes, C. E., & Xue, Z. L. (1999). Investigation of uranyl adsorption on mesoporous titanium-based sorbents. Radiochim. Acta. 84, 37-42.

NUCLEAR MATERIALS

Actinide (Heavy Element) Chemistry

Project: 59967

Title: Aqueous Electrochemical Mechanisms in Actinide Residue Processing

PI: Dr. David E. Morris *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Morris, D. E. (1998, Jul. 27-30). Aqueous electrochemical mechanisms in actinide residue processing. DOE Environmental Management Science Program Workshop. Chicago, IL.

Morris, D. E. (1999, Apr. 21-25). Trends in actinyl electrochemistry: Voltammetry and theory. Presentation at the 217th National Meeting of the American Chemical Society. Anaheim, CA.

Morris, D. E. (1999, Aug. 22-26). Aqueous electrochemical mechanisms in mediated dissolution of actinide residues. First Accomplishments of Environmental Management Science Program. National Meeting of the American Chemical Society. New Orleans, LA.

Morris, D. E. (1999, Aug. 22-26). Aqueous electrochemical mechanisms in actinide residue processing results. Presentation at the National Meeting of the American Chemical Society. New Orleans, LA.