

HIGH-LEVEL WASTE

Actinide (Heavy Element) Chemistry

Project: 59977

Title: Synthesis and Characterization of Templated Ion Exchange Resins for the Selective Complexation of Actinide Ions

PI: Dr. George M. Murray

Institution: Johns Hopkins University
Applied Physics Lab

Publication Type: Journal

Bae, S. Y., Southard, G. L., & Murray, G. M., (1999 Oct. 4). Molecularly imprinted ion exchange resin for purification, preconcentration, and determination of UO₂²⁺ by spectrophotometry and plasma spectrometry. *Anal. Chim. Acta.* 397(1-3), 173-181.

Publication Type: Paper

Arnold, B. R., Jenkins, A. L., Uy, O. M., & Murray, G. M. (1999). Progress in the development of molecularly imprinted polymer sensors. *JHUAPL Technical Digest.* 20, 190-198.

Publication Type: Presentation

Kimaro, A. & Murray, G. M. (1998, Mar. 7-12). Synthesis and characterization of templated ion exchange resins for the selective complexation of actinide ions. Abstract No. 2315P, Pittsburgh Conference. Orlando, FL.

Project: 65370

Title: Actinide-Specific Interfacial Chemistry of Monolayer Coated Mesoporous Ceramics

PI: Dr. Glen E. Fryxell

Institution: Pacific Northwest National
Laboratory

Publication Type: Journal

Feng, X., et. al. (1999). Self-assembled monolayers on mesoporous silica, a super sponge for actinides. In Mara, J. C. & Chandler, G. T. (Eds.), *Ceramic Transactions, 93, Environmental Issues and Waste Management Technologies IV.* 35-42.

Fryxell, G. E., et. al. (1999, Aug.). Design and synthesis of selective mesoporous anion traps. *Chem. Mater.* 11(8), 2148-2154.

Fryxell, G. E., Liu, J., & Mattigod, S. V. (1999, Dec.). Self-assembled monolayers on mesoporous supports (SAMMS) - an innovative environmental sorbent. *Mater. Technol.* 14(4), 188-191.

Publication Type: Other

Fryxell, G. E. & Liu, J. (1999, in press). Designing surface chemistry in mesoporous silica. In Papirer, E. (Ed.), Adsorption at Silica Surfaces. Marcel Dekker.

Publication Type: Presentation

Fryxell, G. E., et al. (1999, Jun.). Self-assembled monolayers on mesoporous supports: Synthesis of nanoscale hybrid materials and their applications. Presentation at the Northwestern Regional Meeting of the American Ceramic Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Apr.). Design and synthesis of mesoporous lanthanide sorbent materials. Invited presentation at the 101st National Meeting of the American Ceramic Society.

Fryxell, G. E., et. al. (1999, Apr.). Environmental applications of interfacially modified mesoporous ceramics. Invited presentation at the 101st National Meeting of the American Ceramic Society.

Fryxell, G. E., et. al. (1999, Aug.). Environmental applications of Self-Assembled Monolayers on Mesoporous Supports (SAMMS). Invited presentation at the National Meeting of the American Ceramic Society. New Orleans, LA.

Fryxell, G. E., et. al. (1999, Jun.). High efficiency environmental sorbent materials: Self-assembled Monolayers on Mesoporous Support (SAMMS) for metal removal from aqueous systems. Presentation at the Symposium on Environmental Chemistry at the Northwestern Regional Meeting of the American Chemical Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Jun.). High efficiency environmental sorbent materials: Self-assembled Monolayers on Mesoporous Supports (SAMMS) for metal removal from aqueous systems. Presentation at the Northwestern Regional Meeting of the American Ceramic Society. Portland, OR.

Fryxell, G. E., et. al. (1999, Jun.). Self assembled monolayers on mesoporous supports: Synthesis of nanoscale hybrid materials and their applications. Presentation at the Symposium on Nanoscale Materials at the Northwestern Regional Meeting of the American Chemical Society. Portland, OR.

Fryxell, G. E., Zemanian, T. S., & Yin, Y. H. (1999, Aug. 22). Environmental applications of self-assembled monolayers on mesoporous supports. Abstr. Pap. Am. Chem. S. 218, U1089-U1089, Part 1.

Publication Type: Press release

Fryxell, G. E. (1999, Apr. 11). PNNL focuses on healthy environment. Tri-City Herald, D1.

Fryxell, G. E. (1999, Mar.). Metal eaters. Popular Science, 34.

Project: 73749 (Renewal of Project No. 54621)

Title: Chemical Speciation of Strontium, Americium, and Curium in High Level Waste:
Predictive Modeling of Phase Partitioning During Tank Processing

PI: Dr. Andrew R. Felmy *Institution:* Pacific Northwest National
Laboratory

Publication Type: Journal

Felmy, A. R. & Mason, M. J. (1998). The displacement of strontium from organic chelates by hydroxide, carbonate, and calcium in concentrated electrolytes. *Journal of Solution Chemistry*. 27(5), 435-454.

Felmy, A. R. & Rai, D. (1999, May). Application of Pitzer's equations for modeling the aqueous thermodynamics of actinide species in natural waters: A review. *J. Solution Chem.* 28(5), 533-553.

Felmy, A. R., Dixon, D. A., Rustad, J. R., Mason, M. J. & Onishi, L. M. (1998). The hydrolysis and carbonate complexation of strontium and calcium in aqueous electrolytes: Use of molecular modeling calculations in the development of aqueous thermodynamic models. *J. Chem. Thermodyn.* 30, 1103-1120.

Oakes, C. S., Sterner, S. M. & Felmy, A. R. (2000, Jan.). Thermodynamic properties of aqueous calcium nitrate [Ca(NO₃)₂] to the temperature 373K including new enthalpy of dilution data. *J. Chem. Thermodyn.* 32(1), 29-54.

Sterner, S. M., Felmy, A. R., Oakes, C. S., & Pitzer, K. S. (1998). Correlation of thermodynamic data for aqueous electrolyte solutions to very high ionic strength using INSIGHT: Vapor saturated water activity in the system CaCl₂-H₂O to 250 ° C and solid saturation. *International Journal of Thermophysics*. 193, 761-770.

Publication Type: Presentation

Felmy, A. R., Choppin, G. R., Dixon, D. A., & Campbell, J. A. (1998, Jul. 27-30). Chemical speciation of strontium, americium, and curium in high-level waste: Predictive modeling of phase partitioning during tank processing. Two presentations and one poster. Presentations to the Hanford Tanks Site Technology Coordination Group (STCG) on November 10, 1998, and to PNNL staff on January 21, 1998. Poster presentation at the EMSP Principal Investigators Workshop, Chicago, IL.

Felmy, A. R. & Mason, M. J. (1998, Aug. 9-14). The aqueous complexation of Eu(III) with organic chelating agents at high base and high ionic strengths: Metal-chelate displacement induced by hydrolysis and precipitation reactions. 53rd Calorimetry Conference. Midland, MI.

Felmy, A. R., Dixon, D. A. & Mason, M. J. (1997, Aug. 3-8). The complexation of alkaline earth cations by organic chelates at high ionic strength: Competitive effects of hydrolysis and carbonate complexation. 52nd Calorimetry Conference. Asilomar, CA.

Felmy, A. R., Dixon, D. A. & Mason, M. J. (1999, Mar. 21-25). Aqueous complexation of Eu(III) with organic chelating agents at high base concentration: Molecular and thermodynamic modeling results. 217th ACS National Meeting. Anaheim CA.

Felmy, A. R., Dixon, D. A., Campbell, J. A. & Mason, M. J. (1997, Sept. 7-11). The effects of OH, CO₃, and Ca on the displacement of strontium from organic chelates: Implications for waste processing. 214th ACS National Meeting. Las Vegas, NV.

Felmy, A. R., Dixon, D. A., Rustad, J. R., Mason, M. J. & Onishi, L. M. (1997, Aug. 3-8). The use of molecular modeling calculations to improve the development of thermodynamic models: Hydrolysis, carbonate, and EDTA complexation of alkaline earth cations. 52nd Calorimetry Conference. Asilomar, CA.

Oakes, C. S. & Felmy, A. R. (1997, Aug. 3-8). Thermodynamics of [Na₄EDTA+NaOH]{aq}, including new isopiestic measurements, to 373K, 0.1MPa, and stoichiometric ionic strengths of 18.9 mol . kg⁻¹. 52nd Calorimetry Conference, Asilomar, CA.

Oakes, C. S. & Felmy, A. R. (1998, Aug. 9-14). Thermodynamics of [Na₄EDTA+NaOH]{aq}, including new isopiestic and enthalpy of dilution measurements. 53rd Calorimetry Conference. Midland, MI.

Petersen, C. E., Campbell, J. A., Felmy, A. R., Wahl, K. L. & Finch, J. W. (1998, May 31-June 4). Analysis of metal-organic complexes using CE/MS. 46th American Society of Mass Spectrometry Meeting. Orlando, FL.

Sterner, S. M., Felmy, A. R. & Pitzer, K. S. (1997, Jun. 22-27). Correlation of thermodynamic data for aqueous electrolyte solutions to very high ionic strength using INSIGHT: Vapor saturated water activity in the system CaCl₂-H₂O to 250 ° C and solid saturation. Thirteenth Symposium on Thermophysical Properties. Boulder, CO.

Sterner, S. M., Felmy, A. R., Oakes, C. S., Simonson, J. M., & Pitzer, K. (1997, Aug. 3-8). Thermodynamics of aqueous CaCl₂ to 250 ° C, 400 bars and solid saturation. 52nd Calorimetry Conference. Asilomar, CA.

Publication Type: Report

Boger, M. (2001). Results of the MVDSS radiological screening activity were released as a supporting document. RPP-7522, Rev. 0. NHC (376-3355).

Vienna, J. (2001). A PNNL letter report describing the status of studies on the impact of crystallinity on the PCT response of HLW glasses was issued. PNNL (372-2807).

Boger, M. (2001). Mobile variable depth sampling system conceptual design review report. RPP-8147, Rev. 0. NHC (376-3355).

Project: 73759 (Renewal of Project No. 54679)

Title: Computational Design of Metal Ion Sequestering Agents

PI: Dr. Benjamin P. Hay

Institution: Pacific Northwest National
Laboratory

Publication Type: Journal

Bryan, J. C., Delmau, L. H., & Hay, B. P. (1999, Jun.). Cesium recognition by supramolecular assemblies of 2-benzylphenol and 2-benzylphenolate. *Struct. Chem.* 10(3), 187-203.

Bryan, J. C., Sachleben, R. A., & Hay, B. P. (1999, Jun. 30). Structural aspects of cesium ion selectivity by tetrabenzocrown-8. *Inorg. Chim. Acta.* 290(1), 86-94.

Clement, O., Rapko, B. M., & Hay, B. P. (1998). Structural aspects of metal-amide complexes. *Coordination Chemistry Reviews.* 170, 203.

Falana, O. M., Koch, H. R., Roundhill, D. M., Lumetta, G. J., & Hay, B. P. (1998). Synthesis and extraction studies of 1,2- and 1,3-disubstituted butylcalix[4]arene amides with oxyions: Geometric and conformational effects. *Journal of the Chemical Society. Chemical Communications* 503.

Hay, B. P., Clement, O., & Sandrone, G. (1998, Nov. 2). A molecular mechanics (MM3(96)) force field for metal-amide complexes. *Inorg. Chem.* 37(22), 5887-5894.

Hay, B. P., Clement, O., Sandrone, G., & Dixon, D. A. (1998). A MM3(96) force field for metal amide complexes. *Inorganic Chemistry.* 37, 5887.

Koch, H. F., Shen, J., & Roundhill, D. M. (2000). Poly(ethylene) glycol as a selective biphasic phase transfer agent for the extraction of chromium(VI) from aqueous salt solutions. *Separ. Sci. Technol.* 35(4), 623-929.

Koch, H. F., Wolf, N. J., & Roundhill, D. M. (2000). A comparison between the picrate and inductively coupled plasma-atomic emission spectroscopy (ICP-AES) methods of metal assays in solution for calix[4]arene amides and amines as extractants. *Separ. Sci. Technol.* 35(5), 779-784.

Lumetta, G. L., McNamara, B. K., & Rapko, B. M. (1999, Oct. 15). Complexation of uranyl ion by tetrahexyl-malonamides: An equilibrium modeling and infrared spectroscopic study. *Inorg. Chim. Acta.* 293(2), 195-205.

McNamara, B. K., Lumetta, G. J. & Rapko, B. M. (1999). Extraction of europium(III) ion with tetrahexylmalonamides. *Solvent Extr. Ion. Exc.* 17(6), 1403-1421.

Rao, L., Xia, Y., Rapko, B. M., & Martin, P. F. (1998). Synergistic extraction of Eu(III) and Am(III) by thenoyltrifluoroacetone and neutral donor extractants: Octyl(phenyl)-N,N-diisobutylcarbonyl-methylphosphine oxide and 2,6-bis(diphenylphosphino)methyl pyridine N,P,P trioxide. *Solvent Extraction and Ion Exchange.* 16, 913.

Rapko, B. M., McNamara, B. K., Lumetta, G. J., Rogers, R. D., & Hay, B. P. (1999, Oct. 4). Ordination of lanthanide nitrates with N,N,N',N'-tetramethylsuccinamide. *Inorg. Chem.* 38(20), 4585-4592.

Sandrone, G., Dixon, D. A., & Hay, B. P. (1999). Conformational analysis of malonamide, N,N'-dimethylmalonamide, and N,N,N',N'-tetramethylmalonamide. *J. Phys. Chem. A.* 18, 3554.

Sandrone, G., Dixon, D. A., & Hay, B. P. (1999). C(sp²)-C(sp³) rotational barriers in simple amides: H₂N-C(=O)-R, R = methyl, ethyl, i-propyl, t-butyl. *J. Phys. Chem. A.* 103, 893.

Vargas, R., et. al. (2000, Jun. 1). Conformational analysis of N,N,N',N'-tetramethylsuccinamide: The role of C-H center dot center dot center dot O hydrogen bonds. *J. Phys. Chem. A.* 104(21), 5115-5121.

Wolf, N. J., et. al. (1999). Synthesis and crystal structures of lower rim amine and carbamoyl substituted calixarenes as transfer agents for oxyions between an aqueous and a chloroform phase. *Polyhedron.* 18(6), 885-896.

Yordanov, A. & Roundhill, D. M. (1998). Solution extraction of transition and post-heavy and precious metals by chelate and macrocyclic ligands. *Coordination Chemistry Reviews.* 170, 93.

Yordanov, A. T., et. al. (1999). Derivatized calix[4]arenes as selective phase transfer extractants for heavy metal and oxyion salts. *Comments on Inorganic Chemistry.* 20, 163.

Publication Type: Other

Hay, B. P. & Clement, O. (1998). Metal complexes. Invited Book Chapter In Schleyer, P. R., et. al. (Eds.) *The Encyclopedia of Computational Chemistry.* John Wiley and Sons, Chichester, NY.

Publication Type: Presentation

Clement, O., Hay, B. P. Dixon, D. A., & Sandrone, G. (1998, Jun.). A MM3(96) force field for metal-amide complexes. West Coast Theoretical Chemistry Conference. Richland, WA.

Clement, O., Sandrone, G., Dixon, D. A., & Hay, B. P. (1998, Mar.). A MM3(96) force field for metal-amide complexes. 215th American Chemical Society National Meeting, Dallas, TX.

Clement, O., Sandrone, G., Dixon, D. A., & Hay, B. P. (1998, Jun.). A MM3(96) force field for metal-amide complexes. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Hay, B. P. (1998, Aug.). A points-on-a-sphere approach to model metal-ligand interactions with an extended MM3 model. Invited presentation at the 216th American Chemical Society National Meeting, Boston, MA.

Hay, B. P. (1998, Jul.) Architectural design criteria for f-block metal sequestering agents. Environmental Management Science Program Workshop. Chicago, IL.

Hay, B. P. (1998, Oct.) Ligand design with molecular mechanics. INEEL Science Integrated Workshop, Environmental Management Science Program. Idaho Falls, ID.

Hay, B. P. (1999, Jun.) The application of molecular mechanics in the design of metal ion sequestering agents. Invited presentation at the Metal Separation Technologies Beyond 2000: Integrating Novel Chemistry with Processing United Engineering Foundation Conference. Turtle Bay, Oahu, HI.

Hay, B. P., Dixon, D. A., & Sandrone, G. (1998, Jun.) A modified MM3(96) force field for simple amides and diamides. West Coast Theoretical Chemistry Conference. Richland, WA.

Hay, B. P., Dixon, D. A., & Sandrone, G. (1998, Jun.) A modified MM3(96) force field for simple amides and diamides. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Lumetta, G. J., McNamara, B. K., & Burgeson, E. (1997, Jun.) Amide complexes of f-block elements. 21st Annual Actinide Separations Conference. Charleston, SC.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1998, Jun.) Binding of diamide ligands to f-block elements. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1998, Apr.) Binding of amide ligands to f-block elements. 22nd Annual Actinide Separations Conference. Chattanooga, TN.

Lumetta, G. J., McNamara, B. K., & Rapko, B. M. (1999, Mar.) Equilibrium modeling of the extraction of f-block elements by diamides. 217th American Chemical Society National Meeting. Anaheim, CA.

Rao, L., Zanonato, P., & Di Bernardo, P. (1998, Aug.) Thermodynamics of europium(III) complexation with alkyl-substituted diamides in organic solvents. 216th American Chemical Society National Meeting. Boston, MA.

Rapko, B. M. (1997, Apr.) Extraction of f-elements by phosphine oxide/pyridine N-oxide ligands. 213th American Chemical Society National Meeting. San Francisco, CA.

Rapko, B. M., et al. (1999, Mar.) Coordination chemistry of tetraalkyldiamides with f-block metal salts. 217th American Chemical Society National Meeting. Anaheim, CA.

Rapko, B. M., et. al. (1999, Jun.). Coordination chemistry of diamides with f-block metal salts. Metal Separation Technologies Beyond 2000: Integrating Novel Chemistry with Processing United Engineering Foundation Conference. Turtle Bay, Oahu, HI.

Rapko, B. M., Lumetta, G. J., McNamara, B. K., Rao, L., & Zanonato, P. L. (1997, Oct.). Determination of actinide and lanthanide binding constants with amides and diamides. Tenth Symposium on Separation Science and Technology for Energy Applications. Gatlinburg, TN.

Rapko, B. M., McNamara, B. K., Rogers, R. D., Lumetta, G. J., & Hay, B. P. (1998, Jun.). Coordination chemistry of lanthanide salts with N,N,N',N'-tetramethylsuccinamide and N,N,N',N'-tetrahexyl-succinamide. 53rd Northwest Regional American Chemical Society Meeting. Pasco, WA.

Roundhill, D. M. (1998, May). New macrocycles for selective ion exchange. Metals Adsorption Workshop. Cincinnati, OH.

Roundhill, D. M. (1999, Mar.). Calixarene amines and amides as extractants for oxyions. 217th National American Chemical Society National Meeting. Anaheim, CA.

Yordanov, A. T., Wolf, N. J., Koch, H. F., & Roundhill, D. M. (1998, Jun.). Sulfur and nitrogen derivatized calix[4]arenes as selective phase transfer extractants for heavy metals and oxyions. Second Fargo Conference on Main Group Chemistry. Fargo, ND.

Zanonato, P. L. & Rao, L. (1997, Sept.). Complexation of Eu(III) by N,N,N',N'-tetra-alkyldiamides. 214th American Chemical Society National Meeting. Las Vegas, NV.

Publication Type: Proceeding

Hay, B. P. (1999, in press). The use of molecular mechanics in the design of metal ion sequestering agents. In Metal separation technologies beyond 2000: Integrating novel chemistry with processing. United Engineering Foundation. New York, NY.

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1998). Environmental management science program workshop. CONF-980736, Environmental Management Science Program, U.S. Department of Energy, Office of Science and Risk Policy EM-52. Washington, D.C.

Rao, L., Xia, Y., Rapko, B. M., & Martin, P. L. (1997, Jun). Synergistic extraction of Eu(III) and Am(III) by TTA and the neutral donor extractants CMPO and NOPOPO. 21st Annual Actinide Separations Conference. Charleston, SC.

Publication Type: Report

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1997). Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. Fiscal Year 1997 Mid-Year Progress Report. PNNL-11589, Pacific Northwest National Laboratory. Richland, WA.

Hay, B. P., Dixon, D. A., Lumetta, G. J., & Rapko, B. M. (1998). Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. Fiscal Year 1998 Mid-Year Progress Report. PNNL-11899, Pacific Northwest National Laboratory. Richland, WA.

Lumetta, G. J., Rapko, B. M., & McNamara, B. K. (1999). The SX solver: A new computer program for analyzing solvent extraction equilibria. PNNL-12085, Pacific Northwest National Laboratory. Richland, WA.

Project: 81887 (Renewal of Project No. 65411)

Title: Precipitation and Deposition of Aluminum-Containing Phases on Tank Wastes

PI: Dr. Shas Mattigod

Institution: Pacific Northwest National
Laboratory

Publication Type: Proceeding

Liu, J., et. al. (1999, Aug. 22). Characterization of colloidal phases in tank wastes. Abstr. Pap. Am. Chem. S. 218, U1077-U1077, Part 1.

Project: 81896

Title: Speciation, Dissolution, and Redox Reactions of Chromium Relevant to Pre-treatment and Separation of High-level Tank Wastes

PI: Dr. Dhanpat Rai

Institution: Pacific Northwest National
Laboratory

Publication Type: Poster

Rai, D., Rao, L., Clark, S. B., Hess, N. J., & Felmy, A. R. (2000). Speciation, dissolution, and redox reactions of chromium relevant to pretreatment and separation of high-level tank wastes. EMSP National Workshop. Atlanta, GA.

Publication Type: Presentation

Friese, J., et. al. (2000, Mar.). Oxidation of trivalent Cr using oxidants relevant to high-level radioactive waste. 219th American Chemical Society National Meeting. San Francisco, CA.

Friese, J., Ritherdon, B., Clark, S. B., Rao, L., & Zhang, Z. (2001, Apr.). Removing chromium from high-level radioactive waste streams: Speciation and reactivity of Cr(III) oligomers under highly alkaline conditions. 221st American Chemical Society National Meeting. San Diego, CA.

Rai, D., Rao, L., Clark, S. B., Hess, N. J., & Felmy, A. R. (2000, Mar.). Solubility of Cr(III) compounds and their redox transformation reactions: Application to pretreatment of high-level waste sludges. EMSP National Workshop. Atlanta, GA.

Rao, L., et. al. (1999, Aug.). Speciation, dissolution, and redox reactions of Cr(III) in alkaline solutions. 218th American Chemical Society National Meeting. New Orleans, LA.

Rao, L., et. al. (2000, Mar.). Dissolution of Cr(OH)₃(am)/Cr₂O₃(c) and oxidation of Cr(III) in alkaline solutions. 219th American Chemical Society National Meeting. San Francisco, CA.

Publication Type: Report

Rai, D., Rao, L., Clark, S. B., Hess, N. J., & Lumetta, G. J. (2000). Speciation, dissolution, and redox reactions of chromium relevant to pretreatment and separation of high-level tank wastes. In Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Science Program Awards. PNNL-12208. Pacific Northwest National Laboratory. Richland, WA. 1.15-1.17.

Rai, D., Rao, L., Clark, S. B., Hess, N. J., & Lumetta, G. J. (1999). Speciation, dissolution, and redox reactions of chromium relevant to pretreatment and separation of high-level tank wastes. In Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Science Program Awards. PNNL-12208. Pacific Northwest National Laboratory. Richland, WA. 1.61-1.86.

Project: 81962 (Renewal of Project No. 65352)

Title: Understanding the Chemistry of the Actinides in High Level Waste Tank Systems: The Impact of Temperature on Hydrolysis and Complexation with Organics

PI: Dr. Sue B. Clark

Institution: Washington State University

Publication Type: Journal

Clark, S. B. (1999, in press). The aqueous geochemistry of the rare earth elements. IX. A potentiometric study of Nd³⁺ complexation with acetate in 0.1 molal NaCl solutions from 25-225° C. *Geochim. Cosmochim. Acta*.

Yeh, M., Maddison, A., & Clark, S. B. (2000, Mar.). Temperature dependence of chloride complexation for the trivalent f-elements. *J. Radioanal. Nucl. Ch.* 243(3), 645-650.

Yeh, M., Riedener, T., Bray, K., & Clark, S. B. (2000, May 24). A spectroscopic investigation of temperature effects on solution complexation in the Eu³⁺-acetate system. *Journal of Alloys and Compounds*.

Publication Type: Paper

Wood, S. A., Palmer, D. A., Wesolowski, D. J. (1999, Aug. 22-27). Determination of the solubility of crystalline $\text{Nd}(\text{OH})_3$ in sodium triflate solutions from 30 to 250 C with in situ pH measurement. Determination of the solubility of crystalline $\text{Nd}(\text{OH})_3$ in sodium triflate solutions from 30 to 250 C with in situ pH measurement. Ninth Annual V.M. Goldschmidt Conference Abstracts. Harvard University, Cambridge, MA. Lunar and Planetary Institute Contribution No. 791. Houston, TX. 329-330.

Analytical Chemistry & Instrumentation

Project: 55318

Title: Improved Analytical Characterization of Solid Waste Forms by Fundamental Development of Laser Ablation Technology

PI: Dr. Richard E. Russo

Institution: Lawrence Berkeley National Laboratory

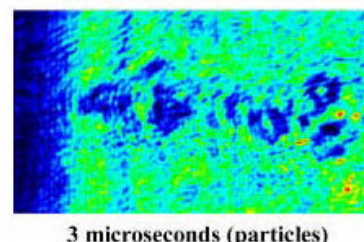
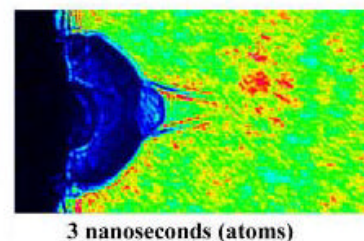
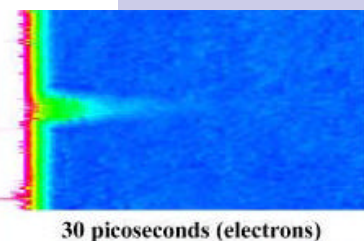
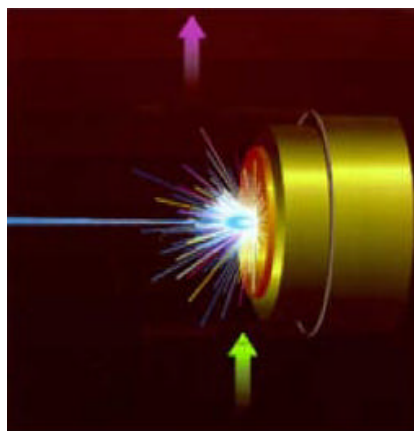
Publication Type: Journal

Borisov, O. V., Mao, X. L., & Russo, R. E. (1999, in press). Laser ablation ICP/MS calibration based on binary Cu/Zn alloy standards. *Spectrochimica Acta B*.

Borisov, O. V., Mao, X. L., Ciocan, A. C., & Russo, R. E. (1998). Time resolved parametric studies of laser ablation using ICP-AES. *Applied Surface Science*. 129, 315.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1998). Effects of gas environment on pico-second laser ablation. *Applied Surface Science*. 129, 269.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1998). Optical emission spectroscopy of the influence of laser ablated mass on dry inductively coupled plasma conditions. *Spectrochimica Acta*. 53B, 463.



Laser ablation is a viable technology for direct characterization of EM solid waste samples. Lawrence Berkeley National Laboratory studied the fundamentals of this technology to assure accuracy of characterization using non matrix-matched standards.

The images at right show ejection of electrons, atoms, and particles at different times during an ablation event. Understanding the contribution of each mass form to the chemical analysis is one of the goals of this research. [see Project #55318]

- Jeong, S. H., Borisov, O. V., Yoo, J. H., Mao, X. L., & Russo, R. E. (1999, Nov. 15). Effects of particle size distribution on inductively coupled plasma mass spectrometry signal intensity during laser ablation of glass samples. *Anal. Chem.* 71(22), 5123-5130.
- Leung, A. P. K., Chan, W. T., Mao, X. L., & Russo, R. E. (1998). Influence of gas atmosphere on picosecond laser ablation sampling efficiency and ICP-AES. *Analytical Chemistry*. 70(N22), 4709.
- Liu, H. C., et. al. (1999, Nov. 8). Early phase laser induced plasma diagnostics and mass removal during single-pulse laser ablation of silicon. *Spectrochim. Acta. B.* 54(11), 1607-1624.
- Russo, R. E. (1998). Laser ablation sampling. *Trends in Analytical Chemistry (Personal Edition)*. 17(8-9).
- Russo, R. E. (1998, Jul. 1). Transient isotachophoretic - electrophoretic separations of lanthanides with indirect laser-induced fluorescence detection. *Analytical Chemistry*. 70(13).
- Russo, R. E. (1998, Jul. 18). Preferential vaporization during laser ablation inductively coupled plasma atomic emission spectroscopy. *Applied Spectroscopy*. 52(7).
- Russo, R. E. (1998, Mar. 30). Optical emission spectroscopy studies of the influence of laser ablated mass on dry inductively coupled plasma conditions. *Spectrochimica Acta, Part B: Atomic Spectroscopy*. 53(3).
- Russo, R. E. (1998, May 29). Enhancements in laser ablation inductively coupled plasma-atomic emission spectrometry based on laser properties and ambient environment. *Spectrochimica Acta, Part B: Atomic Spectroscopy*. 53(5).

Publication Type: Presentation

- Borisov, O. V., Mao, X. L., & Russo, R. E. (1998, Oct.). Optimization of ICPMS for laser ablation sampling. 25th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Austin, TX.
- Chan, W. -T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997, Oct.). Effect of gas medium on laser ablation sampling for ICP-AES. Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies. (FACSS). Providence, RI.
- Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997, Jul.). Effects of gas atmosphere on pico-second laser ablation sampling for ICP-AES. Fourth International Conference on Laser Ablation (COLA 97). Asilomar, CA.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1997, Jul.). Optical emission spectroscopy of the influence of ablated material on dry inductively coupled plasma conditions. COLA 97. Asilomar, CA.

Russo, R. E. (1998, Sept.). Laser-ablation sampling with ICP/AES and ICP/MS: Fundamental issues to improve analytical applications. Invited presentation at the Society of Applied Spectroscopy California Section Meeting. Fremont, CA.

Russo, R. E. (1999, Apr.). Fundamental and applied aspects of laser ablation for chemical analysis. Frontiers in Chemistry Lecture Series. Wayne State University. Detroit, MI.

Russo, R. E., Jeong, S. H., Mao, X. L., Borisov, O. V., & Yoo, J. (1998, Oct.). Particle generation and transport during laser ablation sampling for chemical analysis. 25th Annual Conference of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Austin, TX.

Russo, R. E., Mao, X. L., Ciocan, A. C., & Borisov, B. V. (1997, Oct.). Laser ablation solid sample chemical analysis: Dream or reality. Invited presentation at the Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies (FACSS). Providence, RI.

Russo, R. E., Mao, X. L., Ciocan, A. C., & Borisov, B. V. (1997, Oct.). Laser ablated mass influence on the properties of the ICP. Invited presentation at the Twenty-Fourth Annual Meeting of the Federation of Analytical Chemistry and Spectroscopy Societies. (FACSS). Providence, RI.

Publication Type: Proceeding

Borisov, O. V., Mao, X. L. & Russo, R. E. (1999, Apr.). Direct characterization of solid waste forms using laser ablation ICPMS. Waste Management Science and Technology in the Ceramic and Nuclear Industries. American Ceramic Society.

Chan, W. T., Leung, A. P. K., Mao, X. L., & Russo, R. E. (1997). Effects of gas atmosphere on pico-second laser ablation sampling for ICP-AES. Fourth International Conference on Laser Ablation (COLA 97). Asilomar, CA.

Ciocan, A. C., Mao, X. L., Borisov, O. V., & Russo, R. E. (1997, Jul.). Optical emission spectroscopy studies of ablated material on dry inductively coupled plasma conditions. COLA. Asilomar, CA.

Mao, X. L., Ciocan, A. C., Borisov, O. V., & Russo, R. E. (1997, Jul.). Time resolved parametric studies of laser ablation of brass using ICP-AES. COLA 97. Asilomar, CA.

Russo, R. E. (1997, Jul. 21-25). Effects of gas environment on picosecond laser ablation. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation.

Russo, R. E. (1997, Jul. 21-25). Propagation of the shock wave generated from excimer laser heating of aluminum targets in comparison with ideal blast wave theory. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation.

Russo, R. E. (1997, Jul. 21-25). Time-resolved parametric studies of laser ablation using inductively coupled plasma atomic emission spectroscopy. Applied Surface Science Proceedings of the 1997 4th International Conference on Laser Ablation.

Russo, R. E., Mao, X. L., & Borisov, O. V. (1998). Laser Ablation Sampling. Trends in Analytical Chemistry. 17, 461.

Project: 59978

Title: Thermospray Mass Spectrometry Ionization Processes Fundamental Mechanisms for Speciation, Separation and Characterization of Organic Complexants in DOE Wastes

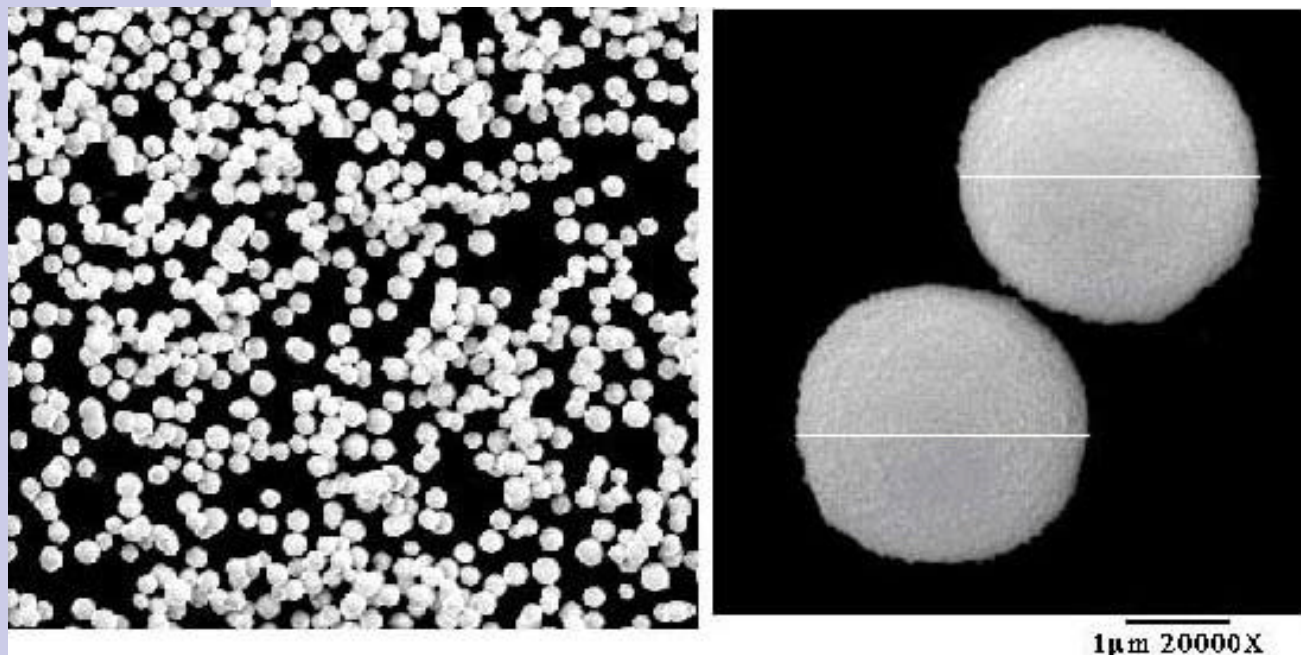
PI: Debra Bostick

Institution: Oak Ridge National Laboratory

Publication Type: Presentation

Bostick, D. (1999, Aug. 22-26). Separation and speciation of organic complexants in DOE wastes using HPLC on zirconia based stationary phases and thermospray mass spectrometry. Presentation at the National Meeting of the American Chemical Society. New Orleans, LA.

Bostick, D. (1999, Nov. 16). HPLC separation of chelating agents on quaternized polyethyleneimine coated zirconia. Eastern Analytical Symposium, Somerset, NJ.



Electron Micrograph of zirconia particles showing uniform particle size. [see Project #59978]

Bostick, D. (2000, Apr. 24-27). Separation and speciation of organic complexants in DOE wastes using HPLC on zirconia-based stationary phases and thermospray mass spectrometry. 2nd Annual Environmental Management Science Program National Workshop, Atlanta, GA.

Caton, J. E. (1998, Jul. 27-30). Thermospray mass spectrometry ionization processes: Fundamental mechanisms for speciation and characterization of organic complexants in DOE wastes. EMSP Workshop. Chicago, IL.

Project: 60075

Title: Particle Generation by Laser Ablation in Support of Chemical Analysis of High Level Mixed Waste from Plutonium Production Operations

PI: Dr. J. Thomas Dickinson *Institution:* Washington State University

Publication Type: Paper

Dickinson, J. T. (1998, Aug.). Mechanisms for and characterization of particulate generation by laser irradiation of inorganic crystalline materials. DOE-EMSP Workshop on Waste Characterization. Chicago, IL.

Dickinson, J. T. (1998, Jun.). Ejection of droplets and fracture particles from single crystal NaNO₃ during pulsed laser irradiation. Gordon Research Conference on Laser Interaction with Materials.

Dickinson, J. T. (1999, Jun.). UV laser interactions with inorganic single crystals with molecular anions. American Chemical Society. Portland, OR.

Dickinson, J. T. (1999, Mar.). High energy ions from UV laser irradiation of cleaved ionic crystals. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). Laser desorption of energetic ions from single crystal NaNO₃ at 1064 nm. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). The effect of surface treatment on excimer laser induced positive ion desorption in brushite. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, Mar.). Ultrafast and nanosecond laser induced desorption from ionic solids. American Physical Society March Meeting. Atlanta, GA.

Dickinson, J. T. (1999, May). Laser-induced positive ion and neutral atom/molecule emission from single crystal CaHPO₄ · 2H₂O: The role of radiation induced defects. Materials Research Society. San Francisco, CA.

Dickinson, J. T. (1999, May). Studies of particulate formation by laser ablation in support of chemical analysis of high level mixed waste. American Ceramics Society. Indianapolis, IN.

Hedges, A. L., Mendoza, A., Alexander, M. L., Langford, S.C., & Dickinson, J. T. (1999, Mar.) Investigations of particle formation by laser ablation for elemental analysis. 217th ACS meeting. Anaheim, CA.

Publication Type: Presentation

Alexander, M. L., Langford, S. C., & Dickinson, J. T. (1998, Oct.). Fundamental mechanisms of particulate formation by laser ablation for inductively coupled plasma mass spectrometry (LA/ICP-MS). Presentation at the SPIE East conference. Boston, MA.

Alexander, M. L., Langford, S.C., & Dickinson, J. T. (1999, Mar.). Particle generation by laser ablation in support of chemical analysis of high level mixed waste from plutonium production operations. Invited presentation at the DOE Characterization and Monitoring Sensor Technology (CMST) meeting. Gaithersburg, MD.

Dickinson, J. T. (1999, Jan.). The desorption of energetic ions from ionic crystals. Dept. of Physics, Washington State University. Pullman, WA.

Dickinson, J. T. (1998, Jun.). The laser desorption of ions from ionic crystals. Gordon Conference on Laser Materials Interactions.

Dickinson, J. T. (1998, Nov.). New models of laser desorption and particle formation. Physics Dept. Colloquium. University of Linz, Austria.

Dickinson, J. T. (1998, Oct. - Nov.). Topics in surface dynamics. Guest Lecturer, Institute of Applied Physics. University of Linz, Austria.

Dickinson, J. T. (1998, Oct.). Mechanisms for and characterization of particulate generation by laser irradiation of inorganic crystalline materials. FACS National Meeting. Austin TX.

Dickinson, J. T. (1999, Jan.). The use of lasers in chemical analysis. University of Minho. Braga, Portugal.

Dickinson, J. T. (1999, Jun.). Laser desorption and chemical analysis. Departments of Physics and Chemistry. U. of Heidelberg, Germany.

Dickinson, J. T. (1999, Jun.). The laser desorption of ions from ionic crystals. E-MRS Symposium on Laser Materials Interactions. Strasbourg, France.

Dickinson, J. T. (1999, Jun.). The use of lasers in chemical analysis of toxic materials. Paul Scherrer Institute. Villigen PSI, Switzerland.

Project: 60219

Title: Development of Advanced Electrochemical Emission Spectroscopy for Monitoring Corrosion in Simulated DOE Liquid Waste

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

Publication Type: Journal

Al-Rifaie, M. & Macdonald, D. D. (2000, in press). On the transients in the thickness of anodic passive films on metals. *J. Electrochem. Soc.*

Engelhardt, G. R. & Macdonald, D. D. (2000, Mar.). Modeling of corrosion fatigue chemistry in sensitized stainless steel in boiling water reactor environments. *CORROSION/2000*, Paper No. 00227 (NACE International, Houston, TX.) Orlando, FL.

Macdonald, D. D. & Heaney, D. F. (1999, May). On the photoinhibition of passivity breakdown on iron in chloride-containing solutions. *J. Electrochem. Soc.* 146(5), 1773-1776.

Macdonald, D. D. (1999). Passivity-the key to our metals-based civilization. *Pure Appl. Chem.* 71(6), 951-978.

Sikora, E. & Macdonald, D. D. (1999, in press). Electrochemical and photoelectrochemical study of passive films on iron formed in the presence of EDTA. *Proc. Int. Symp. Hon. Prof. Norio Sato: Passivity and Localized Corrosion*, Electrochemical Society. Princeton, NJ.

Sikora, J., Sikora, E., & Macdonald, D. D. (2000). The electronic structure of the passive film on tungsten. *Electrochim. Acta.* 45(12), 1875-1883.

Publication Type: Presentation

Liu, J. & Macdonald, D. D. (2000, May 14-19). The passivity of iron in EDTA-containing solutions. *Proc. Electrochem. Soc. 198th Meeting*. Toronto, Canada.

Macdonald, D. D. & Al-Rifaie, M. (2000, May 14-19). New rate law for the anodic growth of passive films. *Proc. Electrochem. Soc. 198th Meeting*. Toronto, Canada.

Macdonald, D. D. & Engelhardt, G. R. (2000, Nov. 19-21). The deterministic prediction of localized corrosion damage. *Corrosion & Prevention 2000*. Auckland, New Zealand.

Macdonald, D. D. (2000, May 14-19). Mechanic analysis by electrochemical impedance spectroscopy. *Proc. Electrochem. Soc. 198th Meeting*. Toronto, Canada.

Macdonald, D. D. (2000, Nov. 19-21). Fundamental aspects of passivity breakdown. *Corrosion & Prevention 2000*. Auckland, New Zealand.

Macdonald, D. D. (2000, Nov. 19-21). Mechanistic analysis by electrochemical impedance spectroscopy. Corrosion & Prevention 2000. Auckland, New Zealand.

Macdonald, D. D., Al-Rifaie, M., & Engelhardt, G. R. (2000, Nov. 19-21). Transient growth and reduction of anodic oxide films on metal surfaces. Corrosion & Prevention 2000. Auckland, New Zealand.

Sikora, E. & Macdonald, D. D. (1999). Electrochemical and photoelectrochemical study of passive films on iron formed in the presence of EDTA. 197th Proc. Electrochem. Soc. Meeting. 99-2(484).

Sikora, J., Sikora, E., & MacDonald, D. D. (1999). Nature of the passive film on tungsten. 197th Proc. Electrochem. Soc. Meeting. 99-2(490).

Project: 65421

Title: Correlation of Chemisorption and Electronic Effects for Metal/Oxide Interfaces: Transducing Principles for Temperature-Programmed Gas Microsensors

PI: Dr. Stephen Semancik

Institution: National Institute of Standards & Technology - Maryland

Publication Type: Patent

Kunt, R. Cavicchi, S. Semancik and T. McAvoy (2001, Aug. 1). Method for Operating a Sensor to Differentiate Between Analytes in a Sample. US #6,095,681

Publication Type: Presentation

Cavicchi, R. E. (1998, Nov. 17). Correlation of chemisorption and electronic effects for metal/oxide interfaces: Transducing principles for temperature programmed gas microsensors. Environmental Management Science Program - Tank Focus Area Workshop. Richland, WA.

Cavicchi, R. E. (1999, Sept. 17-22). Microhotplate gas sensor arrays. Presentation at the SPIE International Symposium on Environmental and Industrial Sensing. Boston, MA.

Ding, J. (1999, Sept. 17-22). Quantification of a single component gas in air with a microhotplate gas sensor using partial least squares techniques. Presentation at the SPIE International Symposium on Industrial and Environmental Sensing. Boston, MA.

McAvoy, T. J. (1999, Aug. 24). Modeling microhotplate gas sensors. Presentation at the ACS National Meeting. New Orleans, LA.

Panchapakesan, B. (1999, Apr. 7). Micromachined array studies of tin oxide films: Nucleation, structure and gas sensing characteristics. MRS Spring National Meeting. San Francisco, CA.

Semancik, S. (1999, Aug. 24). Microarrays as platforms for gas microsensor development and efficient materials research. Presentation at the ACS National Meeting. New Orleans, LA.

Semancik, S. (1999, Sept.). Solid state gas microsensors for environmental and industrial monitoring. Presentation at the SPIE International Symposium on Industrial and Environmental Sensing. Boston, MA.

Walton, R. M. (1999, Jun. 7). Processing methods for selected area film deposition and preparation on microsensor platforms using thermal and potential control. 10th International Conference on Solid-State Sensors and Actuators. Sendai, Japan.

Publication Type: Proceeding

Panchapakesan, B., DeVoe, D. L., Cavicchi, R. E., Walton, R. M., & Semancik, S. (1999, in press). Micromachined array studies of tin oxide films: Nucleation, structure and gas sensing characteristics. Proceedings of the MRS, Spring 1999.

Walton, R., et. al. (1999, Jun.). Processing methods for selected area film deposition and preparation on microsensor platforms using thermal and potential control. Digest 10th International Conference on Solid-State Sensors and Actuators. 1, 676-679. Sendai, Japan.

Project: 65425

Title: Mass Spectrometric Fingerprinting of Tank Waste Using Tunable, Ultrafast Infrared Lasers

PI: Dr. Richard F. Haglund, Jr. *Institution:* Vanderbilt University

Publication Type: Presentation

R. F. Haglund, Jr., (1999, Jun.). The future of tunable, ultrafast lasers in materials analysis and processing. Plenary lecture at the American Society for Mass Spectrometry. Dallas, TX.

Project: 81924 (Renewal of Project No. 60217)

Title: Optical and Microcantilever-Based Sensors for Real-Time In Situ Characterization of High-Level Waste

PI: Dr. Gilbert M. Brown *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Ji, H. - F., Dabestani, R., Brown, G. M., & Hettich, R. L. (1999, Dec.). Optical sensing of cesium using 1,3-alternate calix[4]-mono- and di(anthrylmethyl)aza-crown-6. Photochem. Photobiol. 70(6), 882-886.

Ji, H. -F., Brown, G. M., & Dabestani, R. (1999). Calix[4]arene-based Cs⁺ selective optical sensor. Chem. Comm. 609.

Ji, H. -F., Dabestani, R., Brown, G. M., & Hettich, R. L. (1999). Spacer length effect on the photoinduced electron transfer fluorescent probe for alkali metal ions. *Photochem. Photobiol.* 69, 513.

Ji, H.- F., Dabestani, R., & Brown, G. M. (2000, in press). A supramolecular fluorescent probe activated by protons to detect cesium and potassium ions: An integrated logic gate based on photoinduced electron transfer (PET). *J. Am. Chem. Soc.*

Ji, H.- F., Dabestani, R., Brown, G. M., & Sachleben, R. A. (2000). A new highly selective calix[4]crown-6 fluorescent cesium probe. *J. Chem. Soc. Chem. Comm.* 833.

Publication Type: Presentation

Ji, H. -F., Dabestani, R., & Brown, G. M. (1998, Aug.). Fluorescence probes for the detection of potassium ions. Presentation at the American Chemical Society National Meeting. Boston, MA.

Project: 81939

Title: Hybrid Micro-Electro-Mechanical Systems (MEMS) for Highly Reliable and Selective Characterization of Tank Waste

PI: Dr. Panos G. Datskos

Institution: Oak Ridge National Laboratory

Publication Type: Journal

Betts, T., Tipple, C., Sepaniak, M., & Datskos, P. G. (2000). Selectivity of chemical sensors based on micro-cantilevers coated with polymeric films. *Anal. Chim. Acta.* 422, 89.

Datskos, P. G. & Sauers, I. (2000). Detection of 2-mercaptoethanol using microcantilevers. *Sensors and Actuators B.* 61, 75.

Datskos, P. G. (1999). Chemical detection based on adsorption-induced and photo-induced stresses in MEMS devices. *Detection and Remediation Technologies for Mines and Minelike Targets IV, SPIE,* 3710, 344.

Fagan, B., Xue, B., Datskos, P. G., & Sepaniak, M. (2000, in press). Modification of micro-cantilever sensors with sol-gels to enhance performance and immobilize chemically selective phases. *Talanta.*

Headrick, J., Sepaniak, M., Alexandratos, S., & Datskos, P. G. (2000). Chelating scintillation fibers for measurements of ¹³⁷Cs. *Anal. Chem.* 72, 1994.

Engineering Science

Project: 54656

Title: Mixing Processes in High-Level Waste Tanks

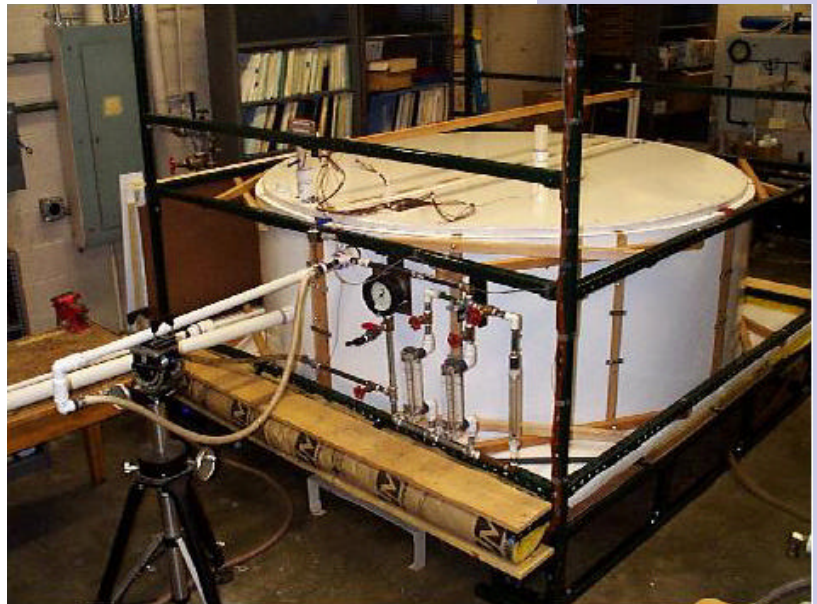
PI: Dr. Per F. Peterson

Institution: University of California at Berkeley

Publication Type: Presentation

Christensen, J. & Peterson, P. F. (1999, Oct. 3-8). A one-dimensional lagrangian model for large-volume mixing. Accepted for the Ninth International Topical Meeting on Nuclear Reactor Thermal Hydraulics. San Francisco, CA.

Kuhn, S. Z., Lee, C., & Peterson, P. F. (1999, Oct. 3-8). Stratification from buoyancy-driven exchange flow through horizontal partitions in a liquid tank. Accepted for the Ninth International Topical Meeting on Nuclear Reactor Thermal Hydraulics. San Francisco, CA.



Study of Mixing and heat-transfer augmentation by injected jets in a large enclosure. [see Project #54656]

Publication Type: Proceeding

Peterson, P. F. & Gamble, R. E. (1998). Scaling for forced-convection augmentation of heat and mass transfer in large enclosures by injected jets. Transactions of American Nuclear Society. 78, 265-266.

Project: 55294

Title: Superconducting Open-Gradient Magnetic Separation for the Pretreatment of Radioactive or Mixed Waste Vitrification Feeds

PI: Richard D. Doctor

Institution: Argonne National Laboratory

Publication Type: Paper

Doctor, R. D. (1997, Oct. 24). Superconducting open-gradient magnetic separation for the pre-treatment of radioactive or mixed-waste vitrification feeds. Tenth Symposium on Separation Science and Technology for Energy Applications.

Project: 60451*Title:* Mechanics of Bubbles in Sludges and Slurries*PI:* Dr. Phillip A. Gauglitz*Institution:* Pacific Northwest National
Laboratory*Publication Type:* Journal

Denn, M. M. & Marrucci, G. (1999, Nov. 15). Squeeze flow between finite plates. *J. Non-Newtonian Fluid.* 87(2-3), 175-178.

Kam, S. I. & Rossen, W. R. (1999, May 15). Anomalous capillary pressure, stress and stability of solids-coated bubbles. *J. Colloid Interf. Sci.* 213(2), 329-339.

Publication Type: Presentation

Gauglitz, P. A., et. al. (1998, Jun.). Mechanics of bubbles in sludges and slurries: Initial progress. Hanford Technical Exchange. Richland, WA.

Gauglitz, P. A., et. al. (1999, Jan.). Mechanics of bubbles in sludges and slurries. Presented at the Hanford Site Technology Coordinating Group - Tank Subgroup. Richland, WA.

Gauglitz, P. A., Terrones, G., Aardahl, C. L., Mendoza, D. P., & Mahoney, L. A. (1999, Mar. 14-19). Mechanics of bubbles in sludges and slurries: Experimental studies and solid mechanics modeling results. Engineering Foundation Conference on Rheology in the Minerals Industry II. Oahu, HI.

Publication Type: Report

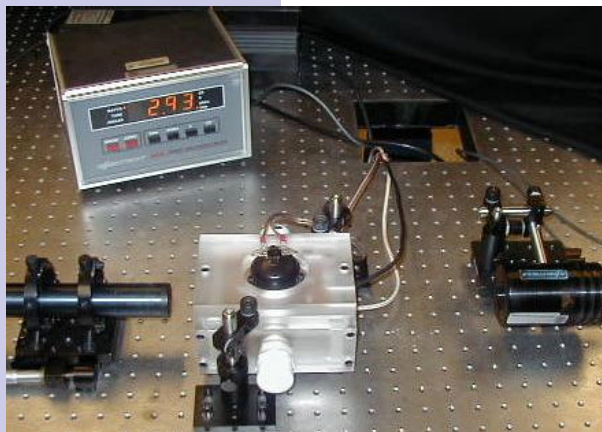
Kam, S. I. (1998). Interactions between bubbles and solids: Three applications. Department of Petroleum and Geosystems Engineering. The University of Texas. Austin, TX.

Project: 65328*Title:* Electrically Driven Technologies for Radioactive Aerosol Abatement*PI:* Dr. David W. DePaoli*Institution:* Oak Ridge National Laboratory*Publication Type:* Journal

Carter, J. & Ezekoye, O. A. (2000, in press). Design of an oscillating flow apparatus for the study of low-Reynolds-number particle dynamics. *Experiments in Fluids.*

Publication Type: Presentation

Ezekoye, O. A. (1998, Nov. 17-18). Electrically driven technologies for radioactive aerosol abatement. EMSP/TFA Workshop, Richland, WA.



Particle interactions in electric and acoustic fields are studied in a unit reactor. [see Project #65328]

Schmidt, J. J., et. al. (2000, Apr. 24-27). Electrically driven technologies for radioactive aerosol abatement. Presentation at the 2nd Annual Environmental Management Science Program National Workshop, Atlanta, GA.

Wibowo, Y. W. & Ezekoye, O. A. (1999, Sep.). Computations of sedimentation rates for acoustically enhanced agglomeration. AIChE CCPS Annual International Conference and Workshop on Modeling Consequences of Accidental Releases of Hazardous Materials, San Francisco, CA.

Publication Type: Theses/Dissertations

Carter, J. (2000). Study of fluid oscillation and its effect on low Reynolds number particle sedimentation. M. S. Thesis, University of Texas at Austin, TX.

Lakshminarasimhan, K. (in progress). Electrically driven technologies for radioactive aerosol abatement. M. S. Thesis, University of Texas at Austin, TX.

Riahi-Nezhad, C. (projected 2001). Electrically driven technologies for radioactive aerosol abatement. M. S. Thesis, University of Tennessee, Knoxville, TN.

Schmidt, J. J. (2000). Experimental study of electrocoalescence in a unit reactor. M. S. Thesis, University of Texas at Austin, TX.

Project: 65371

Title: Numerical Modeling of Mixing of Chemically Reacting, Non-Newtonian Slurry for Tank Waste Retrieval

PI: Dr. David A. Yuen

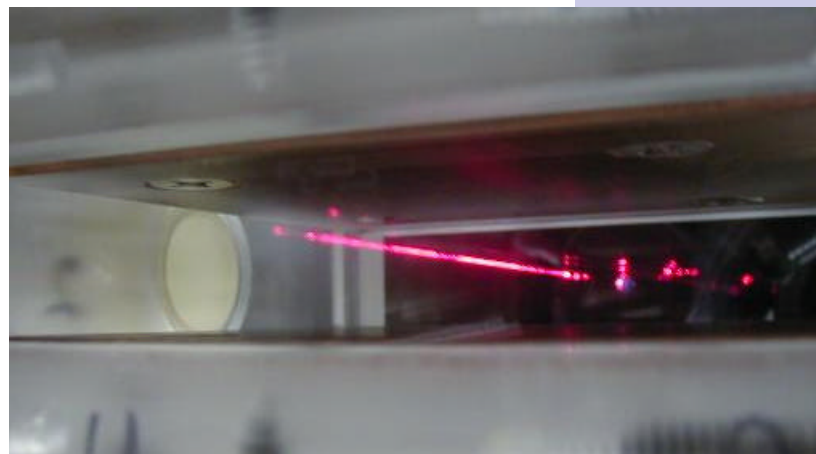
Institution: University of Minnesota

Publication Type: Journal

Ten, A. A., Podladchikov, Y. Y., Yuen, D. A., Larsen, T. B., & Malevsky, A. V. (1998). Comparison of mixing properties in convection with the particle-line method. *Geophys. Res. Lett.* 25(16), 3205-3208.



Experimental apparatus allows testing of the effect of electric and acoustic fields on flowing aerosols in 10-cm (4-inch) square duct. Size distribution and concentration of aerosol are measured to determine effectiveness of agglomeration. [see Project #65328]



Particle size distribution and concentration are measured by light scattering. [see Project #65328]

Ten, A. A., Yuen, D. A. & Podladchikov, Y. Y. (1999, in press). Numerical modeling of mixing of chemically reacting, non-Newtonian slurry for tank waste retrieval. *Electronic Geosciences*.

Publication Type: Proceeding

Onishi, Y. & Trent, D. S. (1999, Mar. 14-19). Mobilization modeling of erosion-resisting radioactive tank waste. *Proceedings of Rheology in the Mineral Industry II*, Kahuku, Oahu, HI. Organized by United Engineering Foundation. New York, NY. 45-56.

Onishi, Y., Trent, D. S., Michener, T. E., Van Beek, J. E., & Rieck, C. A. (1999, Jul. 18-23). Simulation of radioactive tank waste mixing with chemical reactions. FEDSM99-7786: *Proceedings of 3rd ASME/JSME Joint Fluids Engineering Conference*. San Francisco, CA.

Project: 73896 (Renewal of Project No. 55179)

Title: Acoustic Monitor for Liquid-Solid Slurries Measurements at Low Weight Fractions

PI: Dr. Lawrence L. Tavlarides *Institution:* Syracuse University

Publication Type: Journal

Spelt, P. D. M., Norato, M. A., Sangani, A. S., & Tavlarides, L. L. (1999, May). Determination of particle size distributions from acoustic wave propagation measurements. *Phys. Fluids*. 11(5), 1065-1080.

Geochemistry

Project: 73859 (Renewal of Project No. 55042)

Title: Quantify Silica Reactivity in Subsurface Environments: An Integrated Experimental Study of Quartz and Amorphous Silica to Establish a Baseline for Glass Durability

PI: Dr. Patricia M. Dove *Institution:* Virginia Polytechnic Institute & State Univ.

Publication Type: Other

Dove, P. M. & Icenhower, J. (1997). Kinetic and thermodynamic controls on silica reactivity: An analog for waste disposal media. *Commissariat a L' Energie Atomique - Valhro, Ecole D'ete*. Invited chapter in Gin, S. (Ed.). *Glass: Scientific Research for High Performance Containment*.

Publication Type: Presentation

Dove, P. M. (1997, Aug.). Quantifying silica reactivity in subsurface environments: Controls of Reaction Affinity and Solute Matrix on quartz and SiO₂ glass. *International Nuclear Waste Disposal Conference, CEO-Valhro, France*.

Publication Type: Proceeding

Icenhower, J. & Dove, P. M. (1998). The dissolution kinetics of amorphous silica: Structural controls on reactivity (Abstract). International Mineralogical Association Conference. Toronto, Ontario, Canada.

Hydrogeology

Project: 65410

Title: Rapid Migration of Radionuclides Leaked from High-Level Waste Tanks: A Study of Salinity Gradients, Wetted Path Geometry and Water Vapor Transport

PI: Dr. Anderson L. Ward *Institution:* Pacific Northwest National Laboratory

Publication Type: Presentation

Selker, J. S. (1998, Dec. 5-10). Fingered flow from high salinity sources. Presented at the AGU Fall Meetings. San Francisco, CA.

Ward, A. L. & Gee, G. W. (1999, Oct. 31 - Nov. 4). A numerical analysis of wetting front instability induced by infiltration of highly saline fluids. Symposium on Preferential Flow, Soil Science Society of America Annual Meeting. Salt Lake City, UT.

Inorganic Chemistry

Project: 54628

Title: Colloidal Agglomerates in Tank Sludge: Impact on Waste Processing

PI: Dr. Joel M. Tingey *Institution:* Pacific Northwest National Laboratory

Publication Type: Journal

Liu, J., et. al. (1999, Aug. 22). Characterization of colloidal phases in tank wastes. Abstr. Pap. Am. Chem. S. 218, U1077-U1077, Part 1.

Publication Type: Presentation

Tingey, J. M., Bredt, P. R., & Shekarriz, R. (1999, Mar.). Rheology and settling behavior of Hanford tank wastes and the resulting process streams. Rheology in Mineral Industry II. Kahuku, Oahu, HI.

Tingey, J. M., Bunker, B. C., Graff, G. L., Keefer, K. D., Lea, A. S., & Rector, D. R. (1998, Nov.). Colloidal agglomerates in tank sludge and their impact on waste processing. Materials Research Society Fall Meeting. Boston, MA.

Tingey, J. M., Graff, G. L., & Rector, D. R. (1999, Mar.). Effect of colloidal aggregation on sedimentation and rheology in highly basic, high ionic strength salt solutions. Rheology in Mineral Industry II. Kahuku, Oahu, HI.

Project: 54765

Title: Enhanced Sludge Processing of HLW: Hydrothermal Oxidation of Chromium, Technetium, and Complexants by Nitrate

PI: Dr. Stephen J. Buelow

Institution: Los Alamos National Laboratory

Publication Type: Journal

Goemans, M. G. E., Funk, T. J., Sedillo, M. A., Buelow, S. J., & Anderson, G. K. (1997). Electrical conductances of aqueous solutions of inorganic nitrates at 25-505_C and 100-490 bar. *Journal of Supercritical Fluids*, 11, 61-72.

Publication Type: Presentation

Buckley, B., et. al. (1998, Mar. 9-12). Dissolution of chromium oxide under hydrothermal conditions. Presentation at the AIChE 1998 Spring Meeting, New Orleans, LA.

Buelow, S. J. (1996, Oct.). Hydrothermal processing of TRU contaminated wastes. Presentation at the Third International Conference on Oxidation Technologies, Cincinnati, OH.

Buelow, S. J. (1998, Feb. 26-27). Hydrothermal processing of high risk wastes. Presentation at the SCWO Short Course, Supercritical Water Oxidation—Engineering Solutions—Effective Wastewater Treatment and Sludge Management, University of Texas, Austin, TX.

Buelow, S. J., et. al. (1999, Aug. 22-26). Oxidative dissolution of chromium hydroxide by oxygen under hydrothermal conditions. Presentation at the ACS 1999 Fall Meeting, New Orleans, LA.

Ding, Z. Y., et. al. (1998, Jul. 27-30). Enhanced sludge processing of HLW: Hydrothermal Oxidation of Chromium. Presentation at the Environmental Management Science Program Workshop, Rosemont, IL.

Goemans, M. G. E., Butenhoff, T. J., Gloyna, E. F., Anderson, G. K., & Buelow, S. J. (1997, Jun. 22-27). Molecular diffusion of inorganic nitrate species and ketones in subcritical and supercritical water. Presentation at the Thirteenth Symposium on Thermophysical Properties, Boulder, CO.

Mosher, T., Ding, Z. Y., Buelow, S. J., Foy, B. R., & Robinson, J. M. (1997, Nov. 16-21). Dissolution of chromium oxide in hydrothermal conditions by nitrate. Presentation at the AIChE 1997 Annual Meeting, Los Angeles, CA.

Project: 73778 (Renewal of Project No. 60296)

Title: Research Program to Investigate the Fundamental Chemistry of Technetium

PI: Dr. David K. Shuh

Institution: Lawrence Berkeley National Laboratory

Publication Type: Presentation

Amonette, A. B., et. al. (1999). The removal of pertechnetate anions from simulated aqueous radioactive tank wastes using supported zero-valent iron. American Chemical Society National Meeting. New Orleans, LA.

Burns, C. J., Fickes, M. G., & Scott, B. L. (1999). Development of synthetic strategies for the preparation of Tc complexes potentially relevant to tank waste and of methodology to immobilize Tc on solid supports. American Chemical Society National Meeting. New Orleans, LA.

Edelstein, N. E. (1998). Aqueous technetium chemistry. U. S. Department of Energy Technetium Workshop. Pacific Northwest National Laboratory. Richland, WA.

Edelstein, N. M. (1999, Sept. 22-25). Technetium chemistry in highly basic solutions. Presentation at the Technetium Chemistry Workshop. Hanford, WA.

Edelstein, N. M., et. al. (1998). Research program to investigate the fundamental chemistry of technetium. Environmental Management Science Program Workshop. Chicago, IL.

Lukens, W. W., Allen, P. G., Bucher, J. J., Edelstein, M. N., & Shuh, D. K. (2000). Radiation chemistry of technetium in highly alkaline solution. Environmental Management Science Program Workshop. Atlanta, GA.

Lukens, W. W., Allen, P. G., Bucher, J. J., Edelstein, M. N., & Shuh, D. K. (2000). Radiation chemistry of technetium in highly alkaline solution. American Chemical Society Meeting. San Francisco, CA.

Lukens, W. W., Bucher, J. J., Edelstein, M. N., & Shuh, D. K. (2000). Radiation chemistry of technetium in highly alkaline solution. American Chemical Society Western Regional Meeting. San Francisco, CA.

Lukens, W. W., et. al. (1999). The chemistry of reduced technetium in base. American Chemical Society National Meeting. New Orleans, LA.

Mallouk, T. E., et. al. (2000). Some chemical solutions to the remediation of aqueous wastes containing cesium, technetium, and other toxic metal ions. Environmental Management Science Program Workshop. Atlanta, GA.

Shuh, D. K. (1998). Radionuclide environmental chemistry. Department of Chemistry. Foothill College. Los Altos, CA.

Shuh, D. K. (1998). Synchrotron radiation techniques for the investigation of environmental materials science. MRS Spring Meeting. San Francisco, CA.

Shuh, D. K. (1998). Technetium chemistry in cement waste forms. U. S. Department of Energy Technetium Workshop. Pacific Northwest National Laboratory. Richland, WA.

Project: 73832 (Renewal of Project No. 55229)*Title:* The NO_x System in Homogeneous and Heterogeneous Nuclear Waste*PI:* Dr. Dan Meisel*Institution:* University of Notre Dame*Publication Type:* Journal

Cook, A. R., et. al. (2001, Mar. 16). Reducing radicals in nitrate solutions: The NO₃²⁻ system revisited. *J. Phys. Chem. B*, 105. Web Edition.

Dimitrijevic, N. M., Henglein, A., & Meisel, D. (1999). Charge separation across the silica nanoparticle/ water interface. *J. Phys. Chem. B*. 103, 7073-7076.

Fessenden, R. W., Meisel, D., & Camaioni, D. M. (2000). Addition of oxide radical ions (O⁻) to nitrite and oxide ions (O₂⁻) to nitrogen dioxide. *J. Am. Chem. Soc.* 122, 3773-3774.

Schatz, T., Cook, A., & Meisel, D. (1999). Capture of charge carriers at the silica nanoparticle - water interface. *J. Phys. Chem. B*, 103. 10209-10213.

Publication Type: Presentation

Schatz, T., Cook, A. R., & Meisel, D. (1998). Charge carrier transfer across the silica nanoparticle / water interface. *J. Phys. Chem. B*. 102, 7225-7230.

Publication Type: Proceeding

Babad, H. & Camaioni, D. M. (2000, Feb. 27-Mar. 2). The aging of organic chemicals in Hanford high-level wastes. Tucson, AZ.

Meisel, D. (1997). Semiconductor nanoclusters, physical, chemical, and catalytic aspects. In Kamat, P. V. & Meisel, D. (Eds.), *Studies in Surface Science and Catalysis*. 103, 79-97.

Meisel, D. (2000). Radiation induced charge carriers in aqueous suspensions of nanoparticles. *Proceedings of the Trombay Symposium on Radiation and Photochemistry. II*, 271-279.

Meisel, D., Camaioni, D., & Orlando, T. (2001). Radiation and chemistry in nuclear waste: The nox sytem and organic aging. In Eller, G. & Heineman, W. R. (Eds.), *ACS Symposium Series 778*. 342-361.

Meisel, D., Cook, A., Camaioni, D., & Orlando, T. (1997). Photoelectrochemistry. In Rajeshwar, K., Peter, L. M., Fujishima, A., Meissner, D., & Tomkiewicz, M. (Eds.), *The Electrochemical Society Pub.* 97-20, 350-357.

Orlando, T. & Meisel, D. (2001). Radiation-induced processes in aqueous suspensions of nanoparticles and nanoscale water films. In Eller, G. & Heineman, W. R. (Eds.), *ACS Symposium Series 778*. 284-296.

Materials Science

Project: 54773

Title: Microstructural Properties of High-Level Waste Concentrates and Gels with Raman and Infrared Spectroscopies

PI: Dr. Stephen F. Agnew *Institution:* Los Alamos National Laboratory

Publication Type: Presentation

Agnew, S. (1997, Jun. 18-21). IR and raman studies of high level waste concentrates. Presentation at the 52nd Northwest Regional ACS Meeting, Moscow, ID.

Johnston, C. (1999, Mar. 11). Microstructural properties of high level waste concentrates and gels with raman and infrared spectroscopies. Presentation at the CMST-CP annual review conference, Gaithersburg, MD.

Project: 55188

Title: Chemical Decomposition of High-Level Nuclear Waste Storage/Disposal Glasses Under Irradiation

PI: Dr. David L. Griscom *Institution:* Naval Research Laboratory

Publication Type: Journal

Griscom, D. L., Beltran-Lopez, V., Merzbacher, C. I., & Bolden, E. (1999, Jul. 10-15). Selected papers from the 18th International Congress on Glass, San Francisco, CA. *J. Non-Cryst. Solids*, 253, 1-22.

Griscom, D. L., et. al. (1998). On the structure and radiation chemistry of iron phosphate glasses: New insights from electron spin resonance, Mossbauer, and evolved-gas mass spectroscopy. *Nucl. Inst. & Methods B*, 141, 600-615.

Griscom, D. L., Merzbacher, C. I., Weeks, R. A., & Zuhr, R. A. (1999). Electron spin resonance studies of defect centers induced in a high-level nuclear waste glass simulant by gamma-irradiation and ion-implantation. *J. Non-Cryst. Solids*. 258, 34-47.

Project: 55367

Title: Investigation of Microscopic Radiation Damage in Waste Forms Using ODNMR and AEM Techniques

PI: Dr. Guokui Liu *Institution:* Argonne National Laboratory

Publication Type: Journal

Liu, G. K., et. al. (1998). Crystal-field splitting, magnetic interaction, and vibronic excitations of ^{244}Cm in YPO₄ and LuPO₄. *J. Phys. Chem.* 109, 6800-6808.

Liu, G. K., et. al. (2000). Studies of local structure of Cm³⁺ in borosilicate glass using laser and x-ray spectroscopic methods and computational modeling. *J. Chem. Phys.* 112, 1489-1496.

Liu, G. K., Li, S. T., Beitz, J. V., & Abraham, M. M. (1998). Effects of self-radiation damage on electronic properties of $^{244}\text{Cm}^{3+}$ in an orthophosphate crystal of YPO₄. *J. Alloys & Compounds*. 271/273, 872-875.

Liu, G. K., Zhorin, V. V., Li, S. T., & Beitz, J. V. (2000). Crystal field analysis and Monte Carlo simulation of lattice disordering for Cm^{3+} in YPO₄ and LuPO₄. *J. Chem. Phys.* 112, 373-382.

Zhorin, V. V. & Liu, G. K. (1998). Modeling crystal-field interaction for f-elements in LaC₁₃. *J. Alloys and Compounds* 275/277, 137-141.

Publication Type: Proceeding

G. K. Liu, et. al. (1998). Scientific basis for nuclear waste management XXI. *MRS Sym. Pro.* V506, 921.

Liu, G. K., et. al. (1998). Self-radiation induced anisotropic structure damage in ^{244}Cm -doped orthophosphate LuPO₄. *Scientific Basis for Nuclear Waste Management XXI, Mat. Res. Soc. Symp. Proc.* 506, 921-922.

Project: 59827

Title: The Influence of Radiation and Multivalent Cation Additions on Phase Separation and Crystallization of Glass

PI: Dr. Michael C. Weinberg

Institution: University of Arizona

Publication Type: Journal

Burgner, L. L. & Weinberg, M. C. (2000, Jan.). Crystal nucleation rates in a Na₂O-SiO₂ glass. *J. Non-Cryst. Solids*. 261(1-3), 163-168.

Publication Type: Paper

Jeoung, J. S., Poisl, W. H., Weinberg, M. C., Smith, G. L., & Li, H. (1999). Effect of iron oxidation state on immiscibility temperature in sodium silicate glass. *Amer. Ceram. Soc. Bull.* 78(4), 205.

Project: 65422

Title: Modeling of Spinel Settling in Waste Glass Melter

PI: Dr. Pavel Hrma

Institution: Pacific Northwest National Laboratory

Publication Type: Journal

Casler, D. G. & Hrma, P. (1999). Nonisothermal kinetics of spinel crystallization in a HLW glass. *Mat. Res. Soc. Proc.* 556, 255-262.

Hrma, P., Vienna, J. D., Crum, J. V., Piepel, G. F., & Mika, M. (2000). Liquidus temperature of high-level waste borosilicate glasses with spinel primary phase. *Mat. Res. Soc. Proc.* 608, 671-676.

Izak, P., Hrma, P., Vienna, J. D., & Wilson, B. K. (2001, in press). Effect of oxygen partial pressure on liquidus temperature with spinel primary phase. *Ceram. Trans.*

Izak, P., Hrma, P., Young, J. S., & Klouzek, J. (2001, in press). Evolution of crystalline phases during high-level waste feed-to-glass conversion. *Ceram. Trans.*

Klouzek, J., Alton, J., Plaisted, T. J., & Hrma, P. (2001, in press). Crucible study of spinel settling in high-level waste glass. *Ceram. Trans.*

Mika, M., Hrma, P., & Schweiger, M. J. (2000). Rheology of spinel sludge in molten glass. *Ceramics-Silikaty*. 44, 86-90.

Plaisted, T. J., Alton, J., Wilson, B. K., & Hrma, P. (2001, in press). Effect of minor component addition on spinel crystallization in simulated high-level waste glass. *Ceram. Trans.*

Plaisted, T. J., Hrma, P., Vienna, J., & Jiricka, A. (2000). Liquidus temperature and primary crystallization phases in high-zirconia high-level waste borosilicate glasses. *Mat. Res. Soc. Proc.* 608, 706-714.

Plaisted, T. J., Mo, F., Wilson, B. K., & Hrma, P. (2001, in press). Surface crystallization of spinel and acmite in high-level waste glass. *Ceram. Trans.*

Stachnik, M. W., Hrma, P., & Li, H. (2000). Effects of high-level waste glass composition on spinel precipitation. *Ceram. Trans.* 107, 123-130.

Publication Type: Paper

Mika, M., Crum, J. V., & Hrma, P. (1999). Spinel precipitation in high-level waste glass. *Proceedings of the 5th ESG Conference*. Prague, Czech Republic.

Publication Type: Presentation

Hrma, P. & Alton, J. (2001). Dissolution and growth of spinel crystals in high-level waste glass: Diffusion coefficient and boundary layer thickness. *ICEM '01. The 8th International Conference on Radioactive Waste Management and Environmental Remediation*. Bruges, Belgium.

Hrma, P. & Vienna, J. D. (2000). Balancing cost and risk by optimizing the high-level waste and low-activity waste vitrification. *Waste Management '00*. University of Arizona. Tuscon, AZ.

Hrma, P., Izak, P., Klouzek, J., Mika, M., Nemeč, L., & Schill, P. (1999, Aug. 22). Chemistry and hydrodynamics of spinel settling in molten glass. *Abstr. Pap. Am. Chem. S.* 218, U1080-U1080, Part 1.

Izak, P., Hrma, P., & Schweiger, M. J. (1999, Aug. 22). Nonisothermal crystallization of spinel from a high-level waste feed. Abstr. Pap. Am. Chem. S. 218, U1081-U1081, Part 1.

Izak, P., Hrma, P., & Schweiger, M. J. (2001). Kinetics of conversion of high-level waste to glass. ACS Symp. Series. 778, 314-328.

Matyas, J., Klouzek, J., Nemeč, L., & Trochta, M. (2001). Spinel settling in HLW melter. ICEM '01. The 8th International Conference on Radioactive Waste Management and Environmental Remediation. Bruges, Belgium.

Schill, P. (1999, Aug. 22). A three-dimensional mathematical model of radioactive waste glass melter. Abstr. Pap. Am. Chem. S. 218, U1077-U1077, Part 1.

Schill, P. (1999, Aug. 22-26). 3-D mathematical model of radioactive waste glass melter. 218th American Chemical Society National Meeting. New Orleans, LA.

Schill, P., Franek, A., Trochta, M., & Viktorin, P. (1999, Oct. 3-6). Integrated glass furnace model. Glass and Optical Materials Division Fall Meeting. Cleveland, OH.

Publication Type: Proceeding

Hrma, P., et. al. (2001). Increasing high-level waste loading in glass without changing the baseline melter technology. Waste Management '01. University of Arizona. Tucson, AZ.

Schill, P., Trochta, M., Matyas, J., Nemeč, L., & Hrma, P. (2001). Mathematical model of spinel settling in a real waste glass melter. Waste Management '01. University of Arizona. Tucson, AZ.

Schill, P., Trochta, M., Matyas, J., Nemeč, L., & Hrma, P. (2001). Mathematical model of spinel settling in a real waste glass melter. Waste Management Symposium 2001. Tucson, AZ.

Wilson, B. K., Plaisted, T. J., Alton, J., & Hrma, P. (2001, in press). The effect of composition on spinel equilibrium and crystal size in high-level waste glass. TMS Proc.

Publication Type: Report

Hrma, P. (1999). Modeling of spinel settling in waste glass melter. In Science to Support DOE Site Cleanup. Pacific Northwest National Laboratory. PNNL-12208 UC-2000.

Publication Type: Theses/Dissertations

Matyas, J. (2001). Description of the behavior of multitude particles in non-isothermal convective melting space. PhD. Dissertation. Laboratory of Inorganic Materials. Prague, Czech Republic.

Project: 73748 (Renewal of Project No. 60345)

Title: New Metal Niobate and Silicotitanate Ion Exchangers: Development and Characterization

PI: Yali Su

Institution: Pacific Northwest National Laboratory

Publication Type: Journal

Nyman M., et. al. (1999, in press). Synthesis and characterization of a new microporous Cs-Ti-Si-O-H₂O ion exchanger. *Chemistry of Materials*.

Nyman, M., et. al. (1999, Mar. 21). Synthesis, characterization, ion exchange, and ion selectivity of novel microporous Cs-Na-Si-Ti-X-O-H₂O (X=transition metal) materials. *Abstr. Pap. Am. Chem. S.* 217, U924-U924, Part 1.

Xu, H. W., Navrotsky, A., Nyman, M. D., & Nenoff, T. M. (2000, Mar.). Thermochemistry of microporous silicotitanate phases in the Na₂O-Cs₂O-SiO₂-TiO₂-H₂O system. *J. Mater. Res.* 15(3), 815-823.

Publication Type: Patent

Balmer, M. L. (2000, Jan. 14). Novel niobate based molecular sieves. Pending.

Publication Type: Presentation

Balmer, M. L. (1999). Results on phases a, b (Si, Ti phases) and e, f (Niobate phases). *United Engineering Foundations: Metals Separations for 2000 and beyond*.

Balmer, M. L., et. al. (1999, Apr. 25-28). Ceramic wasteforms from Cs-loaded crystalline silicotitanates. *101th Annual Meeting of the American Ceramic Society*. Indianapolis, IN.

Nyman, M. D. & Nenoff, T. M. (1999, Jun.). Selective inorganic crystalline ion exchange materials for cesium and strontium. *United Engineering Foundation and AIChE*.

Nyman, M. D., et. al. (1998). CSTs: Stability and use as alternative waste forms. *Mat. Res. Soc. Fall Meeting*.

Nyman, M. D., et. al. (1999). Hydrothermal synthesis of Cs-Ti-Si-O phases as alternative waste forms for Cs-loaded CST ion exchangers. *1999 Spring American Chemical Society Meeting*. Anaheim, CA.

Su, Y., et. al. (1998). Evaluation of thermally converted silicotitanate waste forms II. *Mat. Res. Soc. Fall Meeting*.

Xu, H., et. al. (1999, Apr. 25-28). Thermo-chemistry of crystalline silicotitanate phases in the Cs₂O-Na₂O-SiO₂-TiO₂-H₂O system. *101st Annual Meeting of the American Ceramic Society*. Indianapolis, IN.

Publication Type: Proceeding

Nyman, M. D., et. al. (1998). CSTs: Stability and use as alternative waste forms. Proc. Mat. Res. Soc. Fall Meeting.

Project: 73750 (Renewal of Project No. 54672)

Title: Radiation Effects in Nuclear Waste Materials

PI: Dr. William J. Weber

Institution: Pacific Northwest National
Laboratory

Publication Type: Journal

Begg, B. D., Hess, N. J., & Weber, W. J. (2000, Apr.). XAS and XRD study of annealed Pu-238- and Pu-239-substituted zircons ($Zr_{0.92}Pu_{0.08}SiO_4$). J. Nucl. Mater. 278(2-3), 212-224.

Corrales, L. R. (1999, Jun. 21). The formation and migration energetics of radical defects in silica polymorphs. Abstr. Pap. Am. Chem. S. 217, U293-U293, Part 2.

Gorretta, K. C., et. al. (1999). Solid-particle erosion of Portland cement and concrete. Wear 224, 106-112.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). U and Pu LIII XAFS of Pu-doped glass and ceramic waste forms. Journal of Alloys and Compounds, 271-273, 240-243.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. Journal of Nuclear Materials. 254, 175-184.

Park, B., Weber, W. J., & Corrales, L. R. (2000). Molecular dynamics study of the threshold displacement energy in MgO. Nucl. Instrum. and Methods, B, 166-167, 357-363.

Song, J., Jonsson, H., & Corrales, L. R. (2000). Self-trapped excitons in quartz. Nucl. Instrum. and Methods, B, 166-167, 451-458.

Thevuthasan, S., Jiang, W., & Young, J. S. (2000, Mar.). Investigation of thermal recovery behavior in hydrogen-implanted SrTiO₃ using high energy ion beam techniques. Nucl. Instrum. Meth. B. 161, 544-548.

Weber, W. J., Ewing, R. C., & Meldrum, A. (1997). The kinetics of alpha-decay-induced amorphization in zircon and apatite containing weapons-grade plutonium or other actinides. Journal of Nuclear Materials. 250, 147-155.

Williford, R. E., Begg, B. D., Weber, W. J., & Hess, N. J. (2000, Apr.). Computer simulation of Pu 3+ and Pu 4+ substitutions in zircon. J. Nucl. Mater. 278(2-3), 207-211.

Williford, R. E., Devanathan, R., & Weber, W. J. (1998). Computer simulation of displacement threshold energies for several ceramic materials. *Nuclear Instruments and Methods B*. 141, 98-103.

Williford, R. E., Weber, W. J., Devanathan, R., & Cormack, A. N. (1999, Jul.). Native vacancy migrations in zircon. *J. Nucl. Mater.* 273(2), 164-170.

Publication Type: Other

Begg, B. D., et. al. (1999, in press). Heavy-ion irradiation effects in pyrochlores. Smith, G. L., Chandler, G. T., & Mobasher, B. (Eds.), *Waste Management Science and Technology in the Ceramic and Nuclear Industries*. The American Ceramic Society. Westerville, OH.

Chen, X., Birtcher, R. C., & Donnelly, S. E. (1999). Bubble formation and growth in glasses. Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.). *Microstructural Processes in Irradiated Materials*. Mater. Res. Soc. Symp. Proc. 540. Warrendale, PA. 331-336.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jonsson, H. (2000). A comparative study of oxygen vacancy migration pathways in crystalline polymorphs of silica. Chandler, G. T. & Feng, X. (Eds). *Environmental Issues and Waste Management Technologies in the Ceramic and Nuclear Industries V*, *Ceramics Transactions*, Westerville, OH. 107, 139-150.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, in press). Vacancy migration and excitons in silica polymorphs. Smith, G. L., Chandler, G. T., & Mobasher, B. (Eds.). *Mater. Waste Management Science and Technology in the Ceramic and Nuclear Industries*. The American Ceramic Society. Westerville, OH.

Publication Type: Paper

Williford, R. E. & Weber, W. J. (1999, Apr. 25-28). Defect formation and migration energetics in disordered Gd₂Ti₂O₇. The 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Publication Type: Presentation

Begg, B. D., et. al. (1999, Apr. 25-28). Heavy-ion irradiation effects in pyrochlores. The 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Begg, B. D., Hess, N. J., & Weber, W. J. (1999, Apr. 22-23). XAS and XRD characterization of annealed Pu-doped zircon. CEA Meeting on HLW and Pu Immobilization. Saclay, France.

Chen, X., Birtcher, R. C., & Donnelly, S. E. (1998, Nov. 30 - Dec. 4). Bubble formation and growth in nuclear waste glasses. Materials Research Society Annual Meeting. Boston, MA.

Corrales, L. R. & Song, J. (1997, Sept.). Molecular dynamics simulations of excitons in glasses. CEA/VALHRO Summer School. Mejanne le Clap, France.

Corrales, L. R. (1997, Oct.). Lattice theories and molecular dynamics simulations of glasses. Department of Chemistry, University of Maryland. College Park, MD.

Corrales, L. R. (1997, Oct.). Molecular dynamics simulations of defects and excitons in glasses. American Ceramics Society, Glass and Optical Materials Division Meeting. Williamsburg, VA.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, Apr. 25-28). The formation and migration energetics of radical defects in silica polymorphs. Invited presentation at the 101st Meeting of The American Ceramic Society. Indianapolis, IN.

Corrales, L. R., Song, J., VanGinhoven, R. M., & Jónsson, H. (1999, Mar. 21-25). Migration of oxygen vacancy radical defects and self-trapped excitons in silica. Invited presentation at the 217th American Chemical Society Meeting. Anaheim, CA.

Corrales, L. R., VanGinhoven, R. M., Song, J., & Jónsson, H. (1998, Nov. 30 - Dec. 4). Vacancy migration barrier energetics and pathways in silica. Materials Research Society Annual Meeting. Boston, MA.

Devanathan, R., Weber, W. J., & Boatner, L. A. (1997, Dec. 1-5). Response of zircon to electron and Ne + irradiation. Materials Research Society Annual Meeting. Boston, MA.

Devanathan, R., Weber, W. J., & Williford, R. E. (1998, Nov. 30 - Dec. 4). Amorphization of Gd₂Ti₂O₇ by energetic heavy ion irradiation. Materials Research Society Annual Meeting. Boston, MA.

Fortner, J. A., Hanchar, J. M., Badyal, Y., Price, D. L., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Structural analysis of a completely amorphous 238 Pu-doped zircon by neutron diffraction. Materials Research Society Annual Meeting. Boston, MA.

Hess, N. J., Maupin, G. D., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Spectroscopic studies of gamma-irradiated glass waste forms. Materials Research Society Annual Meeting, Boston, MA.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1997, Sept. 21-26). U and Pu LIII XAFS of Pu-doped glass and ceramic waste forms. International Conference on Actinides '97. Baden-Baden, Germany.

Song, J. & Corrales L. R. (1998, Mar. 16-20). Simulation of exciton processes in networked materials. March APS National Meeting. Anaheim, CA.

- Song, J., Corrales, L. R., & Jónsson, H. (1998, Nov. 30 - Dec. 4). Exploring the excited states of vacancy defects in silica. Materials Research Society Annual Meeting. Boston, MA.
- Thevuthasan, S., Jiang, W., McCready, D. E., & Weber, W. J. (1998, Nov. 30 - Dec. 4). Damage accumulation and thermal recovery in SrTiO₃ implanted with various ions. Materials Research Society Annual Meeting. Boston, MA.
- Weber, W. J. & Corrales, L. R. (1998, July 27-30). Radiation effects in nuclear waste forms. DOE Environmental Management Science Program Scientific Workshop. Rosemont, IL.
- Weber, W. J. & Devanathan, R. (1998, May 4-6). Effects of alpha decay on crystalline ceramic waste forms. American Ceramic Society Meeting. Cincinnati, OH.
- Weber, W. J. (1988, July 27-30). EMSP projects in materials science. DOE Environmental Management Science Program Scientific Workshop. Rosemont, IL.
- Weber, W. J. (1997, Dec. 1). Radiation effects in glass and ceramic waste forms. Invited presentation at the Massachusetts Institute of Technology. Cambridge, MA.
- Weber, W. J. (1997, Dec. 11). Radiation effects in glass waste forms. Invited presentation at Argonne National Laboratory. Argonne, IL.
- Weber, W. J. (1997, Feb. 20). Radiation effects from the incorporation of plutonium in glasses and ceramics. Invited presentation at Los Alamos National Laboratory. Los Alamos, NM.
- Weber, W. J. (1998, Apr. 19-22). Effects of radiation on solid nuclear waste forms. Invited plenary lecture at the DOE Workshop on Research Needs and Opportunities in Radiation Chemistry. Chesterton, IN.
- Weber, W. J. (1998, Apr. 3-4). Radiation effects from alpha decay in nuclear waste ceramics. Invited plenary lecture at the American Nuclear Society Northern Student Conference. Ann Arbor, MI.
- Weber, W. J. (1998, Jan. 8). Radiation effects in crystalline waste form phases. Invited presentation at the Idaho National Engineering and Environmental Laboratory. Idaho Falls, ID.
- Weber, W. J., et. al. (1998, Nov. 30 - Dec. 4). The effect of temperature and recoil spectra on amorphization in zircon. Materials Research Society Annual Meeting. Boston, MA.
- Weber, W. J., Ewing, R. C., & Meldrum, A. (1998, Mar. 30 - Apr. 3). Radiation effects in nuclear waste ceramics. American Chemical Society Annual Meeting. Dallas, TX.

Weber, W. J., Hess, N. J., Conradson, S. D., & Vienna, J. D. (1997, Aug. 25-27). Self-radiation effects in glass and ceramic waste forms for the stabilization and disposition of plutonium. Topical Conference on Plutonium Futures - The Science. Santa Fe, NM.

Williford, R. E., Devanathan, R. & Weber, W. J. (1997, Sept. 14-19). Computer simulation of displacement threshold energies for several ceramic materials. 9th International Conference on Radiation Effects in Insulators. Knoxville, TN.

Williford, R. E., Weber, W. J., Devanathan, R., & Gale, J. D. (1998, Nov. 30 - Dec. 4). Oxygen vacancy migration in $Gd_2(Ti,Zr)_2O_7$ pyrochlores. Materials Research Society Annual Meeting. Boston, MA.

Publication Type: Proceeding

Corrales, L. R. & Song, J. (1998). Semi-empirical methodology to simulate exciton processes in glasses. Proceeds of the CEA/VALRHO Summer School on Glass: Scientific Research for High Performance Containment. CEA/Valrhô, Bagnols-sur-Cèze, France, 218-227.

Corrales, L. R., VanGinhoven, R. M., Song, J., & Jónsson, H. (1999). Vacancy migration barrier energetics and pathways in silica. Bulatov, V. V., Diaz de la Rubia, T., Phillips, R., Kaxiras, E., & Ghoniem, N. (Eds.) Multiscale Modeling of Materials. Mater. Res. Soc. Symp. Proc. 538, Warrendale, PA. 317-321.

Devanathan, R., Weber, W. J., & Boatner, L. A. (1998). Response of zircon to electron and Ne + irradiation. Ma, E., Bellon, P., Atzmon, M., & Trivedi, R. (Eds.) Phase Transformations and Systems Driven far from Equilibrium. Mater. Res. Soc. Symp. Proc. 481, Warrendale, PA. 419-424.

Fortner, J. A., Hanchar, J. M., Badyal, Y., Price, D. L., & Weber, W. J. (1999, in press). Structural analysis of a completely amorphous ^{238}Pu -doped zircon by neutron diffraction. Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.). Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Heinisch, H. L., Williford, R. E. & Weber, W. J. (1998, Nov. 30 - Dec. 4). Computer simulations of irradiation-induced defect accumulation and amorphization in zircon. Materials Research Society Annual Meeting. Boston, MA.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1998). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. McKinley, I. G. & McCombie, C. (Eds.), Scientific Basis for Nuclear Waste Management XXI. Mater. Res. Soc. Symp. Proc. 506, Warrendale, PA. 169-176.

Hess, N. J., Weber, W. J., & Conradson, S. D. (1997, Sept. 28 - Oct. 3). X-ray absorption fine structure of aged, Pu-doped glass and ceramic waste forms. MRS Symposium, Scientific Basis for Nuclear Waste Management XXI. Davos, Switzerland.

Thevuthasan, S., Jiang, W., McCready, D. E., & Weber, W. J. (1999, in press). Damage accumulation and thermal recovery in SrTiO₃ implanted with various ions. Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Weber, W. J., et. al. (1999, in press). The effect of temperature and recoil spectra on amorphization in zircon. Zinkle, S. J., Ewing, R. C., Lucas, G. E., & Williams, J. S. (Eds.), Microstructural Processes in Irradiated Materials. Mater. Res. Soc. Symp. Proc. 540, Warrendale, PA.

Publication Type: Report

Weber, W. J. & Corrales, L. R. (1997). Radiation effects in nuclear waste materials. Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. PNNL-11589, Pacific Northwest National Laboratory. Richland, WA. 43-52.

Weber, W. J. & Corrales, L. R. (1998). Radiation effects in nuclear waste materials. Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards (PNNL-11889, Pacific Northwest National Laboratory, Richland, WA.). 1.107-1.126.

Weber, W. J. & Corrales, L. R. (1998). Radiation effects in nuclear waste materials. Science to Support DOE Site Cleanup: The Pacific Northwest National Laboratory Environmental Management Science Program Awards. PNNL-11889, Pacific Northwest National Laboratory. Richland, WA. 1.107-1.126.

Weber, W. J., Corrales, L. R., Birtcher, R. C., & Nastasi, M. (1998). Radiation effects in nuclear waste materials. Environmental Management Science Program Workshop (CONF-980736, U. S. Department of Energy, Office of Science and Technical Information, Oak Ridge, TN.). 115-117.

Weber, W. J., Hess, N. J., Conradson, S. D., & Vienna, J. D. (1997). Self-radiation effects in glass and ceramic waste forms for the stabilization and disposition of plutonium. Plutonium Futures - The Science. LA-13338-C, Los Alamos National Laboratory. Los Alamos, NM. 25-26.

Project: 73762 (Renewal of Project No. 54691)

Title: Radiation Effects on Sorption and Mobilization of Radionuclides During Transport Through the Geosphere

PI: Dr. Lu-Min Wang

Institution: University of Michigan

Publication Type: Journal

Gu, B. X., et. al. (2000). The effect of H⁺ irradiation on the Cs ion exchange capacity of zeolite-NaY. *J. Materials Chemistry*. 10, 2610-2616.

Gu, B. X., Wang, L. M., & Ewing, R. C. (2000, Mar.). The effect of amorphization on the Cs ion exchange and retention capacity of zeolite-NaY. *J. Nucl. Mater.* 278, 64-72.

Nyman, M., et. al. (2000). Integrated experimental and computational methods for structure determination and characterization of a new, highly stable cesium silicotitanate phase, Cs₂TiSi₆O₁₅ (SNL-A). *Chemistry of Materials*. 12, 3449-3458.

Nyman, M., Gu, B. X., Wang, L. M., Ewing, R. C., & Neoff, T. M. (2000). Synthesis and characterization of a new microporous cesium silicotitanate (SNL-B) molecular sieve. *Microporous Materials*. 40, 115-125.

Wang, L. M. (1998). Application of advanced transmission electron microscopy techniques in the study of radiation effects in insulators. *Nuclear Instruments and Methods in Physics Research B*. 141, 312-325.

Wang, L. M., Wang, S. X., Gong, W. L., & Ewing, R. C. (1998). Temperature dependence of Kr ion-induced amorphization of mica minerals. *Nuclear Instruments and Methods in Physics Research B*. 141, 501-508.

Wang, S. X., Wang, L. M., & Ewing, R. C. (2000). Electron and ion irradiation of zeolites. *J. Nucl. Mater.* 278, 233-241.

Publication Type: Proceeding

Gu, B. X., Wang, L. M., Simpson, P. A., Minc, L. D., & Ewing, R. C. (2000, in press). Radiation and thermal effects in zeolite-NaY. Smith, R. W. & Shoemith, D. W. (Eds.). *Scientific Basis for Nuclear Waste Management XXIII*, Material Research Society. Warrendale, PA.

Gu, B. X., Wang, S. X., Wang, L. M., & Ewing, R. C. (1999, Aug. 29 - Sept. 3). Radiation and thermal effects on the structure and ion-exchange/retention capacity of zeolites. *Proceedings of the International Conference on the Future Nuclear Systems-Global '99*. American Nuclear Society. Jackson Hole, WY.

Wang, L. M. & Ewing, R. C. (1998, Aug. 31 - Sep. 4). Transmission electron microscopy study of radiation effects in materials for nuclear waste disposal. Benavides, H. A. C. & Yacaman, M. J. (Eds.) *Electron Microscopy 1998, Proceedings of the 14th International Congress on Electron Microscopy*. 2, 825-826. Cancun, Mexico.

Wang, L. M., Wang, X. M., & Ewing, R. C. (1998, May 11-14). Radiation effects in zeolite: Relevance to near-field containment. Proceedings of the 9th Annual International High-Level Radioactive Waste Management Conference, American Nuclear Society. Las Vegas, NV. 772-774.

Wang, S. X., Wang, L. M., & Ewing, R. C. (1999). Electron irradiation of zeolites. Materials Research Society Symposia Proceedings. 540, 361-366.

Project: 73976 (Renewal of Project No. 55110)

Title: Iron Phosphate Glasses: An Alternative for Vitrifying Certain Nuclear Wastes

PI: Dr. Delbert E. Day

Institution: University of Missouri-Rolla

Publication Type: Journal

Badyal, Y., et. al. (2000). The effects of uranium oxide high-level waste on the structure of iron phosphate glasses. MRS 556, 297.

Booth, C. S., et. al. (1999). Oxygen and phosphorus coordination around iron in iron-phosphate glasses with UO₂ or Na₂O and crystalline ferric ferrous pyrophosphate. J. Mat. Res. 14, 2628.

Chen, F. & Day, D. E. (1999). Corrosion of selected refractories by iron phosphate melts. Environment Issues and Waste Management Technologies IV: Ceramic Transactions. 93, 213.

Day, D. E. (1997). Structural features of iron-phosphate glasses. J. Non-Cryst. Solids. 222, 144.

Day, D. E. (1997). Structural study of iron phosphate glasses. Phys. Chem. Glasses. 38, 74.

Day, D. E. (1998). Chemically durable iron phosphate glass wastefoms. J. Non-Cryst. Solids. 241, 1.

Day, D. E. (1998). On the structure and radiation chemistry of iron phosphate glasses: New insights from electron spin resonance and evolved gas mass spectroscopy. Nucl. Inst. Meth. Phys. Res. B. 141, 600.

Day, D. E. (1998). Redox characteristics and structural properties of iron phosphate glasses: A potential host matrix for vitrifying high level nuclear waste. Ceramic Transactions. 87, 261.

Day, D. E. (1999). Effects of nuclear waste components on redox equilibria, structural features, and crystallization characteristics of iron phosphate glasses. Environment Issues and Waste Management Technologies IV: Ceramic Transactions. 93, 195.

Day, D. E. (1999). Iron redox equilibria and crystallization of iron phosphate glasses. Environment Issues and Waste Management Technologies IV: Ceramic Transactions. 93, 187.

Fang, X., Ray, C. S., Marasinghe, G. K., & Day, D. E. (2000). Properties of mixed Na₂O and K₂O iron phosphate glasses. *J. Non-Cryst. Solids* 263, 293.

Karabulut, M., et. al. (1999). X-ray photoelectron and mossbauer spectroscopic studies of iron phosphate glasses containing U, Cs, and Bi. *J. Non-Cryst. Solids*. 249, 106.

Karabulut, M., et. al. (2000). A high-energy x-ray and neutron scattering study of iron-phosphate glasses containing uranium. *J. Appl. Phys.* 87, 2185.

Marasinghe, G. K., et. al. (2000). Properties and structure of vitrified iron phosphate nuclear wasteforms. *J. Non-Cryst. Solids*. 263, 146.

Marasinghe, G. K., et. al. (2000). Vitrified iron phosphate nuclear wasteforms containing multiple waste components. *Environment Issues and Waste Management Technologies V: Ceramic Transactions*. 107, 115.

Mesko, M. G. & Day, D. E. (1999). Immobilization of spent nuclear fuel in iron phosphate glass. *J. Nuclear Matls.* 273, 27-36.

Mesko, M. G., Day, D. E., & Bunker, B. C. (2000). Immobilization of CsCl and SrF₂ in iron phosphate glass. *Environment Issues and Waste Management Technologies V: Ceramic Transactions*. 107.

Mogus-Milankovic, A., Day, D. E., & Santic, B. (1999). DC conductivity and polarization in iron phosphate glasses. *Phys. Chem. Glasses* 40 (2),69-74.

Mogus-Milankovic, A., Santic, B., Pivac, B., & Day, D. E. (1999). TSC and DC conductivity for cesium iron phosphate glasses. *Phys. Chem. Glasses* 40(6), 305-310.

Ray, C. S., Fang, X., Karabulut, M., Marasinghe, G. K., & Day, D. E. (1999). Effects of melting temperature and time on iron valence and crystallization of iron phosphate glasses. *J. Non-Cryst. Solids*. 249, 1.

Project: 81934 (Renewal of Project No. 60020)

Title: Stability of High Level Radioactive Waste Forms

PI: Dr. Theodore M. Besmann *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Allendorf, M. D. & Spear, K. E. (2000, in press). Mechanisms of silica refractory corrosion in glass-melting furnaces: Equilibrium predictions. *J. Electrochem. Soc.*

Besmann, T. M., Beahm, E. C., & Spear, K. E. (1999). An approach to thermochemical modeling of nuclear waste glass. Marra, J. C. & Chandler, G. T. (Eds.), *Environment Issues and Waste Management Technologies IV*, 277-87. *Ceramic Transactions*, 93. American Ceramic Society. Westerville, OH.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1998). Thermochemical modeling of nuclear waste glass. Hou, P. Y., McNallan, M.J., Oltra, R., Opila, E. J., & Shores, D. A. (Eds.). High Temperature Corrosion and Materials Chemistry. The Electrochemical Society, 10 South Main St. Pennington, NJ. 98-9, 512-523.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1999, Apr. 11). Thermochemical modeling of glass: Application to high-level nuclear waste glass. MRS Bulletin. Germany. 24(4), 37-44.

Spear, K. E., Palmisiano, M. N., Pantano, C. G., Besmann, T. M., & Beahm, E. C. (1999). Surface modification of glass by vaporization reactions. Mountziaris, T. J., et. al. (Eds.). Proceeding Symposium Fundamental Gas-Phase and Surface Chemistry of Vapor-Phase Materials Synthesis. The Electrochemical Society, 10 South Main St. Pennington, NJ. 98-23, 388-394.

Publication Type: Presentation

Besmann, T. M., Beahm, E. C., & Spear, K. E. (1998, May 6). An approach to thermochemical modeling of high-level nuclear waste glass. 100th annual meeting of the American Ceramic Society. Cincinnati, OH.

Spear, K. E. (1998, 20 May). Thermochemical modeling applied to glass processes in industry and nuclear waste processes. Chemistry Division Seminar, NIST. Gaithersburg, MD.

Spear, K. E. (1998, Nov. 30 - Dec. 4). Thermochemical models of liquid solutions in nuclear waste glass subsystems. Materials Research Society Fall Meeting.

Spear, K. E. (1998, Oct. 15). Thermodynamic and kinetic modeling capabilities. 75 Years of Ceramics at Penn State, and the 53rd annual PCA Forum. Penn State. University Park, PA.

Spear, K. E. (1999, Apr. 25-28). Solid solution thermochemical models for phase systems in high-level nuclear waste glass. 101st annual meeting of the American Ceramic Society.

Spear, K. E. (1999, Dec. 21). A predictive thermodynamic model for glass: Applications to high-level radioactive waste. Seminar at Northeastern University (New England Local Section of ECS), Boston, MA.

Spear, K. E. (2000, Feb. 23). A predictive thermodynamic model for glass: Applications to high-level radioactive waste, corrosion in glass, furnaces, and float glass processing. Seminar at IIT (Local Section of ECS), Chicago, IL.

Spear, K. E. (2000, May 4). Theory and applications of a thermodynamic model for glass. Seminar at Georgia Tech (Local Section of ECS), Atlanta, GA.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1998, May 7). A thermochemical modeling of nuclear waste glass. Symposium on High Temperature Corrosion and Materials Chemistry. 193rd meeting of the Electrochemical Society. San Diego, CA.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (1998, Jul. 22). Thermodynamic modeling of nuclear waste glass. Gordon Research Conference on High Temperature Materials Chemistry and Diagnostics. Plymouth, NH.

Spear, K. E., Besmann, T. M., & Trowbridge, L. D. (2000, Aug. 6-11). Thermochemical modeling of high-level nuclear waste glass. IUPAC-Sponsored Sixteenth International Conference on Chemical Thermodynamics (ICCT-2000), Tenth International Symposium on Thermodynamics of Nuclear Materials (STNM-2000), Halifax, NS, Canada.

Spear, K. E., Palmisiano, M. N., Pantano, C. G., Besmann, T. M., & Beahm, E. C. (1998, Nov. 6). Surface modification of glass by vaporization reactions. Symposium on the Fundamental Gas-Phase and Surface Chemistry of Vapor-Phase Materials Synthesis. The Electrochemical Society Meeting. Boston, MA.

Publication Type: Proceeding

Besmann, T. M., Spear, K. E., & Beahm, E. C. (2000). Thermochemical models for nuclear waste glass subsystems - MgO-CaO and MgO-Al₂O₃. Materials Research Society.

Spear, K. E. & Allendorf, M. D. (2000). Mechanisms of silica refractory corrosion in glass-melting furnaces: Equilibrium predictions. McNallan, M., Opila, E., Maruyama, T., & Narita, T. (Eds). High Temperature Corrosion and Materials Chemistry: Per Kofstad Memorial Symposium. The Electrochemical Society, Pennington, NJ. Proc. Vol. 99-38.

Spear, K. E., Besmann, T. M., & Beahm, E. C. (2000, Apr. 11). Thermochemical modeling of glass: Application to high-level nuclear waste glass. 10th International Conference on High Temperature Materials Chemistry (HTMC X). Julich, Germany.

Project: 81963 (Renewal of Project No. 65366)

Title: Physical, Chemical and Structural Evolution of Zeolite - Containing Waster Forms Produced from Metakaolinite and Calcined Sodium Bearing Waste

PI: Dr. Michael W. Grutzeck

Institution: Pennsylvania State University

Publication Type: Proceeding

Siemer, D. D., Grutzeck, M. W., & Scheetz, B. E. (1999, Apr. 25-28). Comparison of materials for making hydroceramic waste forms. Proc. Amer. Ceram. Soc. Symposium on Waste Management Science and Technology in the Ceramic and Nuclear Industries, Indianapolis, IN. American Ceramic Society. Westerville, OH.

Separations Chemistry

Project: 54716

Title: Polyoxometalates for Radioactive Waste Treatment

PI: Dr. Michael T. Pope

Institution: Georgetown University

Publication Type: Journal

Dickman, M. H., Gama, G. J., Kim, K. -C., & Pope, M. T. (1996). The structures of europium(III)- and uranium(IV) derivatives of $[P_5W_{30}O_{110}]^{15-}$. Evidence for Cryptohydration. *J. Cluster Sci.* 7, 67-583.

Kim, K. -C. & Pope, M. T. (1999, Sep. 22). Cation-directed structure changes in polyoxometalate chemistry. Equilibria between isomers of bis(9-tungstophosphatodioxouranate(VI)) complexes. *J. Am. Chem. Soc.* 121(37), 8512-8517.

Kim, K. C., et. al. (1999, Dec. 8). Slow proton exchange in aqueous solution. Consequences of protonation and hydration within the central cavity of Preyssler anion derivatives. $[-M(H_2O)-GP_5W_{30}O_{110}]^{(n-)}$. *J. Am. Chem. Soc.* 121(48), 11164-11170.

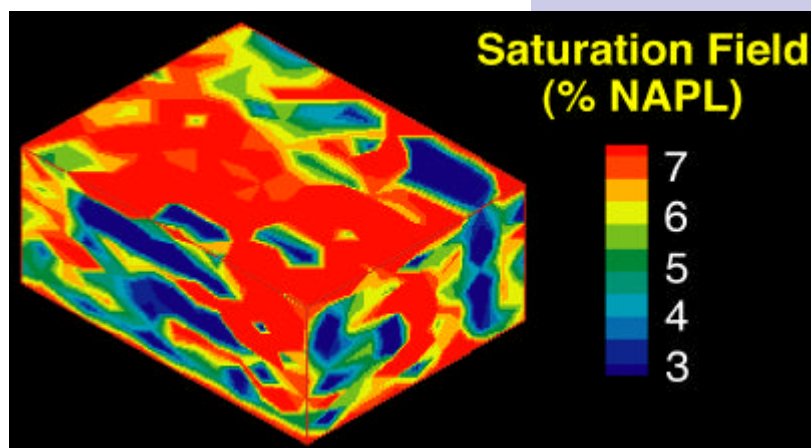
Müller, A., Peters, F., Pope, M. T., & Gatteschi, D. (1998). Polyoxometalates: Very large structures - nanoscale magnets. *Chem. Rev.* 98, 239-271.

Pope, M. T., Wei, X., Wassermann, K., & Dickman, M. H. (1998). New developments in the chemistry of heteropolytungstates of rhodium and cerium. *C. R. Acad. Sci. 1. Ser. IIc*, 297-304.

Wassermann, K., Dickman, M. H., & Pope, M. T. (1997). Self-assembly of supramolecular polyoxometalates. The compact, water-soluble heteropolytungstate anion $[As^{III}_{12}Ce^{III}_{16}(H_2O)_{36}W_{148}O_{524}]^{76-}$. *Angew. Chem.* 109, 1513-1516.

Publication Type: Patent

Pope, M. T., Creaser, I. I., & Heckel, M. C. (1997, Apr. 8). Compounds and methods for separation and molecular encapsulation of metal ions. U.S. Patent #5,618,472.



NAPL saturation distribution estimated from partitioning tracer data for the Hill Air Force Base OU1 field test. [see Project #54716]

Project: 54735

Title: Development of Inorganic Ion Exchangers for Nuclear Waste Remediation

PI: Dr. Abraham Clearfield

Institution: Texas A&M University at
College Station

Publication Type: Journal

Khainakov, S. A., et. al. (1999). Hydrothermal synthesis and characterization of alkali metal titanium silicates. *Journal of Materials Chem.* 9, 269-272.

Pertierra, P., Salvado, M. A., Garcia-Granda, S., Bortun, A. I., & Clearfield, A. (1999). Neutron powder diffraction study of $Ti_2(OH)_2OSiO_4 \cdot 1.5H_2O$. *Inorganic Chem.* 38(11), 2563-2566.

Poojary, D. M., Zhang, B., & Clearfield, A. (1998). Synthesis and structures of barium arylbisphosphonates derived from x-ray powder data. *Anales de Quimica Int. Ed.* 94, 401-405.

Sylvester, P. & Clearfield, A. (1999). The removal of strontium from simulated Hanford tank wastes containing complexants. *Separation Science and Technology.* 34(13), 2539-2551.

Sylvester, P., Clearfield, A., & Diaz, R. J. (1999). Pillared montmorillonites: cesium-selective ion-exchange materials. *Science and Technology.* 34(12), 2293-2305.

Trobajo, C., et. al. (1999). Hydrothermal synthesis and ion exchange properties of the novel framework sodium and potassium niobium silicates. *Solvent Extraction and Ion Exchange.* 17(3), 649-675.

Project: 54996

Title: Ionizing Radiation Induced Catalysis on Metal Oxide Particles

PI: Dr. Michael A. Henderson

Institution: Pacific Northwest National
Laboratory

Publication Type: Journal

Alam, M., Henderson, M. A., Kaviratna, P. D., Herman, G. S., & Peden, C. H. F. (1998). Chromyl chloride chemistry at the $TiO_2(110)$ surface. *J. Phys. Chem. B* 102,111.

Epling, W. S., Peden, C. H. F., Henderson, M. A., & Diebold, U. (1998). Evidence for oxygen adatoms on $TiO_2(110)$ resulting from O_2 dissociation at vacancy sites. *Surf. Sci.* 412-413, 333.

Henderson, M. A., et al. (1999). The chemistry of methanol on the $TiO_2(110)$ surface: The influence of vacancies and coadsorbed species. *Faraday Discuss.* 114, 313-329.

Henderson, M. A., et al. (1999, Jun. 24). Interaction of molecular oxygen with the vacuum annealed TiO₂(110) surface: Molecular and dissociative channels. *J. Phys. Chem. B.* 103(25), 5328-5337.

Henderson, M. A., Oreto-Tapia, S., & Castro, M. E. (1998). Electron induced decomposition of CH₃OH on the vacuum annealed surface of TiO₂(110). *Surf. Sci.* 412-413, 252.

Herman, G. S., Gao, Y., Tran, T. T., & Osterwalder, J. (2000). X-ray photoelectron diffraction study of anatase thin film: TiO₂(001). *Surf. Sci.* 447,201.

Herman, G. S., Henderson, M A., Starkweather, K. A., & McDaniel, E. P. (1999, May-Jun.). Mass- spectrometry of recoiled ions, secondary ion mass spectrometry, and Auger electron spectroscopy investigation of Y₂O₃-stabilized ZrO₂(100) and (110). *J. Vac. Sci. Technol. A.* 17(3), 939-944.

Su, Y., et. al. (1998). Gamma-ray destruction of EDTA catalyzed by titania. *J. Adv. Oxid. Technol.* 3, 63.

Taylor, D. P., Simpson, W. C., Knutsen, K., Henderson, M. A., & Orlando, T. M. (1998). Photon stimulated desorption of cations from yttria-stabilized cubic ZrO₂(100). *Appl. Surf. Sci.* 102, 4536.

Publication Type: Poster

Perkins, C. L. (1999). Photoconversion of adsorbed oxygen states on TiO₂(110). The Sixth International Conference on the Structure of Surfaces. Vancouver, British Columbia, Canada.

Publication Type: Presentation

Henderson, M. A. (1997). Application of static secondary ion mass spectrometry in probing the interaction of water with well-defined oxide surfaces. SIMS XI, 11th International Conference on Secondary Ion Mass Spectrometry. Orlando, FL.

Henderson, M. A. (1998). Coadsorption studies with water and oxygen: A small step toward understanding the surface chemical and photochemical properties of TiO₂. Invited presentation at the Department of Chemistry, University of Puerto Rico. Mayaguez, Puerto Rico.

Henderson, M. A. (1998). Coadsorption studies with water: A small step toward understanding the surface chemical and photochemical properties of TiO₂. Invited presentation at the 45th National Symposium of the American Vacuum Society. Baltimore, MA.

Henderson, M. A. (1998). Ionizing radiation induced catalysis: Radiocatalytic degradation of organic contaminants in TiO₂ suspensions. Invited presentation at the Notre Dame Radiation Laboratory, University of Notre Dame. South Bend, IN.

Henderson, M. A. (1998). Probing the surface chemistry of single crystal metal oxides with water. Invited presentation at the 215th National Meeting of the American Chemical Society. Dallas, TX.

Henderson, M. A. (1999). Activation of molecular oxygen on TiO₂(110) by reaction with bridging hydroxyls. First International Workshop on Oxide Surfaces. Elmau, Germany.

Henderson, M. A. (1999). Electron induced decomposition of methanol on the vacuum annealed surface of TiO₂(110). Environmental Molecular Sciences Symposia and First Users' Meeting. Richland, WA.

Henderson, M. A. (1999). The chemistry of methanol on the TiO₂(110) surface: The influence of vacancies and coadsorbed species. Invited presentation at the 114th Faraday Discussion (The Surface Science of Metal Oxides). Ambleside, UK.

Herman, G. S. (1999). Anatase TiO₂ - A structural investigation by x-ray photoelectron diffraction. The Sixth International Conference on the Structure of Surfaces. Vancouver, B. C.

Herman, G. S. (1999). Characterization of oxide surfaces by mass-spectroscopy of recoiled ions. Surface Analysis '99, Applied Surface Symposium, American Vacuum Society. Waukesha, WI.

Peden, C. H. F. (1997, Sept.). The growth, structure, and surface chemistry of oxide films as model surfaces. Invited presentation at the 17th National Congress of the Mexican Surface Science and Vacuum Society. Mazatlan, Mexico.

Peden, C. H. F. (1998, Apr.). Water adsorption and reaction as a probe of oxide surface structure and chemistry. Invited presentation for the Department of Chemistry, Texas A&M University. College Station, TX.

Perkins, C. L. (1999). Interactions of oxygen, water, and defects on the TiO₂(110) surface. Invited presentation at the University of Illinois/Chicago Chemistry Department Seminar. Chicago, IL.

Perkins, C. L. (1999). Photoconversion of adsorbed oxygen states on TiO₂(110). 46th International Symposium of the American Vacuum Society. Seattle, WA.

Perkins, C. L. (1999). Surface chemistries of group IV oxides and borides. Invited presentation at the Washington State University seminar. Richland, WA.

Su, Y. (1997). Radiocatalytic degradation of organic contaminants in colloidal TiO₂ and ZrO₂ suspensions. The Third International Conference on TiO₂ Photocatalytic Purification and Treatment of Water and Air. Orlando, FL.

Su, Y. (1999). Radiocatalytic and photocatalytic studies of oxidation of organics and reduction of water. The 195th Meeting of the Electrochemical Society. Seattle, WA.

Su, Y. (1999). Radiocatalytic degradation of organic contaminants in TiO₂ suspensions. 214th National Meeting of the American Chemical Society. Las Vegas, NV.

Su, Y. (1999, May 2-6). Radiocatalytic and photocatalytic studies of oxidation of organics and reduction of water. The 195th Meeting of the Electrochemical Society, Seattle, WA.

Su, Y. (1999, May 24-28). Radiocatalytic and photocatalytic studies of metal ion reduction and water cleavage into hydrogen. The 5th International Conference on Advanced Oxidation Technologies for Water and Air Remediation, Albuquerque, NM.

Project: 59990

Title: Fundamental Chemistry, Characterization, and Separation of Technetium Complexes in Hanford Waste

PI: Dr. Norman C. Schroeder *Institution:* Los Alamos National Laboratory

Publication Type: Journal

Schroeder, N. C., Ball, J. R., Radzinski, S. D., Whitener, G. D., & Ashley, K. R. (1999). Reillex(TM)-HPQ anion exchange column chromatography: Removal of Per technetate from DSSF-5 simulant at various flow rates. Solvent Extr. Ion Exc. 17(6), 1543-1556.

Publication Type: Other

Schroeder, N. C., Radzinski, S. D., Ashley, K. R., Truong, A. P., & Szczepaniak, P. A. (1998). Technetium oxidation state adjustment for hanford waste processing. Lombardo, N. J. & Schulz, W. W. (Eds.),

Science and Technology for Disposal of Radioactive Tank Waste. Plenum Publishing Corporation. New York, NY.

Publication Type: Proceeding

Ashley, K. R., Whitener, G. D., Schroeder, N. C., Ball, J. R., & Radzinski, S. D. (1999). Bond, A. H., Dietz, M. L. & Rogers, R. D. (Eds.), Progress in Metal Ion Separation and Preconcentration, ACS Symposium Series 716, American Chemical Society. Washington, D. C. 219.

Project: 60017

Title: Removal of Technetium, Carbon Tetrachloride, and Metals from DOE Properties

PI: Dr. Thomas E. Mallouk

Institution: Pennsylvania State University

Publication Type: Journal

Ponder, S. M. & Mallouk, T. E. (1999, Oct.). Recovery of ammonium and cesium ions from aqueous waste streams by sodium tetraphenylborate. *Ind. Eng. Chem. Res.* 38(10), 4007-4010.

Publication Type: Presentation

Ponder, S. M., et. al. (1999, Aug. 22). Ferragels: Supported zero-valent iron as a remediant for aqueous metal ion wastes. *Abstr. Pap. Am. Chem. S.* 218, U1089-U1089, Part 1.

Publication Type: Proceeding

Ponder, S. M., Ford, J. R., Darab, J. G., & Mallouk, T. E. (1999, in press). Ferragels: A new family of materials for remediation of aqueous metal ion solutions. *MRS Symp. Proceedings.*

Project: 60123

Title: Potential-Modulated Intercalation of Alkali Cations into Metal Hexacyanoferrate Coated Electrodes

PI: Dr. Daniel T. Schwartz

Institution: University of Washington

Publication Type: Journal

Haight, S. M., Schwartz, D. T., & Lilga, M. A. (1999). In-situ oxidation state profiling of nickel hexacyanoferrate derivatized electrodes using line-imaging Raman spectroscopy and multivariate calibration. *J. Electrochem. Soc.* 146, 1866.

Project: 60313

Title: Radiation Effects on Transport and Bubble Formation in Silicate Glasses

PI: Dr. Alexander D. Trifunac

Institution: Argonne National Laboratory

Publication Type: Journal

Shkrob, I. A., Tadjikov, B. M., & Trifunac, A. D. (2000, Feb.). Magnetic resonance studies on radiation-induced point defects in mixed oxide glasses. I. Spin centers in B₂O₃ and alkali borate glasses. *J. Non-Cryst. Solids.* 262(1-3), 6-34.

Shkrob, I. A., Tadjikov, B. M., & Trifunac, A. D. (2000, Mar.). Magnetic resonance studies on radiation-induced point defects in mixed oxide glasses. II. Spin centers in alkali silicate glasses. *J. Non-Cryst. Solids.* 262(1-3), 35-65.

Shkrob, I. A., Tadjikov, B. M., Chemerisov, S. D. & Trifunac, A. D. (1999, Sep. 15). Electron trapping and hydrogen atoms in oxide glasses. *J. Chem. Phys.* 111(11), 5124-5140.

Project: 73803 (Renewal of Project No. 55087)

Title: Next Generation Extractants for Cesium Separation from High-Level Waste: From Fundamental Concepts to Site Implementation

PI: Dr. Bruce A. Moyer *Institution:* Oak Ridge National Laboratory

Publication Type: Journal

Bond, A. H., Dietz, M. L., & Chiarizia, R. (2000, in press). Incorporating size-selectivity into synergistic solvent extraction: A review of crown ether-containing systems. *Ind. Eng. Chem. Res.*

Bond, A. H., et. al. (1999). Synergistic solvent extraction of alkaline Earth cations by mixtures of Di-n-octylphosphoric acid and stereoisomers of Dicyclohexano-18-crown-6. *Anal. Chem.* 71, 2757-2765.

Bryan, J. C., et. al. (1999). Cesium recognition by supramolecular assemblies of 2-Benzylphenol and 2-Benzylphenolate. *Structural Chem.* 10(3), 187-203.

Chiarizia, R., et. al. (1999, Aug. 22). Synergistic effects in the extraction of metal ions by mixtures of dialkylphosphoric acids and crown ethers. *Abstr. Pap. Am. Chem. S.* 218, U1049-U1049, Part 1.

Chiarizia, R., Urban, V., Thiyagarajan, P., Bond, A. H., & Dietz, M. L. (2000). Small angle neutron scattering investigation of the species formed in the extraction of Sr(II) by mixtures of Di-n-octylphosphoric acid and dicyclohexano-18-crown-6. *Solvent Extr. Ion Exch.* 18, 451-478.

Dietz, M. L., et. al. (1999). Comparison of column chromatographic and precipitation methods for the purification of a macrocyclic polyether extractant. *Sep. Sci. Technol.* 34, 2943-2956.

Dietz, M. L., et. al. (1999). Ligand reorganization energies as the basis for the design of synergistic metal ion extractants. *J. Chem. Soc., Chem. Commun.* 1177-1178.

Haverlock, T. J., Bonnesen, P. V., Sachleben, R. A., & Moyer, B. A. (2000). Analysis of equilibria in the extraction of cesium nitrate by calix[4]arene-bis(t-octylbenzo-crown-6) in 1,2-dichloroethane. *J. Incl. Phenom. Mol. Recognit. Chem.* 36(1), 21-37.

Hay, B. P. & Nicholas, J. B. (2000, in press). Unexpected binding modes in tetramethoxycalix(4)arene: Implications for ligand design. *J. Am. Chem. Soc.*

Nicholas, J. B. & Hay, B. P. (1999, Dec. 2). Anisole as an ambidentate ligand: Ab initio molecular orbital study of alkali metal cations binding to anisole. *J. Phys. Chem. A.* 100(48), 9815-9820.

Nicholas, J. B., Dixon, D. A., & Hay, B. P. (1999). Ab initio molecular orbital study of cation- π binding between the alkali metal cations and Benzene. *J. Phys. Chem.* 103, 1394-1400.

Sachleben, R. A., et. al. (1999). Dideoxygenated calix[4]arene crown-6 ethers prefer the 1,3-alternate conformation and exhibit enhanced selectivity for cesium over potassium and rubidium. *J. Chem. Soc., Chem. Commun.* 1751-1752.

Sachleben, R. A., et. al. (1999). Surveying the extraction of cesium nitrate by 1,3-alternate calix[4]-arene crown-6 ethers in 1,2-dichloroethane. *Solvent Extr. Ion Exch.* 17(6), 1445-1459.

Publication Type: Media report

Moyer, B. A., et. al. (2000, Feb.). Highlights of technology developed in the chemical separations group. Highlight released to *Chemical Engineering Magazine*. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Publication Type: Presentation

Bond, A. H., Dietz, M. L., Chiarizia, R., & Hay, B. P. (2000, Mar. 26-30). Synergistic extraction of mono-, di-, and trivalent cations by dicyclohexano-18-crown-6 and dialkylphosphoric acids. 219th American Chemical Society National Meeting, San Francisco, CA.

Bond, A. H., Dietz, M. L., Chiarizia, R., Herlinger, A. W., & Hay, B. P. (1999, Aug. 22). Influence of diluent solvation properties on synergistic solvent extraction by dialkylphosphoric acids and dicyclohexano-18-crown-6. 218th American Chemical Society Meeting. New Orleans, LA.

Bond, A. H., et. al. (1998, Aug. 23-27). Synergistic extraction of cations by dicyclohexano-18-crown-6 and dialkyl phosphoric acids in an alcohol diluent. 216th American Chemical Society Meeting. Boston, MA.

Chiarizia, R., Dietz, M. L., Bond, A. H., Hay, B. P., & Moyer, B. A. (1999, Jul. 11). Synergism in the extraction of metal ions by mixtures of organophosphorous acids and substituted crown ethers. International Solvent Extraction Conference (ISEC '99). Barcelona, Spain.

Chiarizia, R., Urban, V., Thiyagarajan, P., Bond, A. H., & Dietz, M. L. (2000, Mar. 26-30). SANS investigations of organic-phase speciation in the extraction of Sr(II) by mixtures of di-n-octylphosphoric acid and dicyclohexano-18-crown-6. 219th American Chemical Society National Meeting, San Francisco, CA.

Delmau, L., Bryan, J. C., Sachleben, R. A., Hay, B. P., & Moyer, B. A. (1999, Mar. 21). Benzyl phenol derivatives: Building blocks for calixarenes. I&EC Symposium on Calixarene Molecules for Separations. 217th American Chemical Society Meeting. Anaheim, CA. Joint sponsorship with the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Dietz, M. L., Bond, A. H., Chiarizia, R., Huber, V. J., Herlinger, A. W., & Hay, B. P. (1999, Aug. 22-26). Synergistic effects in the extraction of metal ions by mixtures of dialkylphosphoric acids and crown ethers. 218th American Chemical Society Meeting. New Orleans, LA.

Dietz, M. L., et. al. (1998, Apr. 2). Synergism in the extraction of cations by mixtures of dialkylphosphoric acids and substituted crown ethers. Abstr. Pap. Am. Chem. S. 215, U666-U667, Part 1.

Dietz, M. L., et. al. (2000, Mar. 26-30). Ligand reorganization energies as a basis for the design of metal ion extraction systems. Invited presentation at the 219th American Chemical Society National Meeting, San Francisco, CA.

Haverlock, T. J., Bonnesen, P. V., Sachleben, R. A., & Moyer, B. A. (1999, Oct. 18-21). The relationship between species and selectivity in the extraction of cesium and potassium nitrate by calix[4]arene-bis(t-octylbenzo-crown-6) in 1,2-dichloroethane. Eleventh Symposium on Separation Science and Technology for Energy Applications. Gatlinburg, TN.

Haverlock, T. J., Bonnesen, P. V., Sachleben, R. A., & Moyer, B. A. (1997, Sept. 7-11). Cs/K selectivity of a lipophilic calix[4]arene-crown-6 extractant in liquid-liquid separations from nitrate media. 214th American Chemical Society National Meeting. Las Vegas, NV.

Hay, B. P. & Nicholas, J. B. (1999, Jul. 22). Calixarene complexes with alkali cations: There is more to binding than you realized. Environmental Molecular Sciences Symposia and First EMSL Users' Meeting. Pacific Northwest National Laboratory. Richland, WA.

Hay, B. P. & Nicholas, J. B. (1999, Mar. 21). Calixarene complexes with alkali cations: There is more to binding than you realized. Invited presentation at the I&EC Symposium on Calixarene Molecules for Separations, 217th American Chemical Society Meeting. Anaheim, CA.

Hay, B. P. (1998, Oct. 20-22). Ligand design with molecular mechanics. INEEL Science Integrated Workshop, Environmental Management Science Program, Idaho Falls, ID.

Hay, B. P., Dietz, M. L., & Horwitz, E. P. (2000, Mar. 26-30). Optimization of the SREX reagent using a molecular mechanics model. Invited presentation at the 219th American Chemical Society National Meeting, San Francisco, CA.

Huber, V. J., Bond, A. H., Chiarizia, R., & Dietz, M. L. (1998, Aug. 23-27). An improved synthesis of individual dicyclohexano crown isomers. 216th American Chemical Society National Meeting. Boston, MA.

Moyer, B. A. (1999, Aug. 22-24). Chemical principles and their use toward remediation of radioactive contamination in wastes and the environment. 218th American Chemical Society National Meeting. New Orleans, LA. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4510000), and the Office of Basic Energy Sciences (KC302020), U. S. Department of Energy.

Moyer, B. A. (1999, Dec. 4). Crown ethers for selective extraction of metal ions: From fundamental to applied chemistry. Invited presentation at Kyoto University, Kyoto, Japan. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A. (1999, Nov. 12). An overview of the R&D in separation science and technology in the USA and future trends: Environmental and waste problems of the USDOE. Invited presentation at Japan Atomic Energy Research Institute (JAERI), Tokai-mura, Ibaraki, Japan. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A. (1999, Nov. 15). Selective extraction of metal ions by crown ethers: Principles and Applications. National Institute for Resources and Environment, Tsubuka, Ibaraki, Japan. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A. (1999, Nov. 17). New separation technologies for rad-waste management: Metal separation processes developed at ORNL. Invited presentation at Japan Atomic Energy Research Institute (JAERI), Tokai-mura, Ibaraki, Japan. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A. (1999, Nov. 19). Principles and applications of crown ethers for selective extraction of metals from wastes. Invited presentation at Himeji Institute of Technology, Himeji, Japan. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A., Bonnesen, P. V., Delmau, L. H., Haverlock, T. J., & Sachleben, R. A. (1998, Sep. 9). Development of an alkaline-side Cs SX process applicable to Savannah River HLW using a calixarene-crown extractant: Interim progress. Solvent Extraction Working Group Meeting for Savannah River HLW, Argonne National Laboratory. Joint sponsorship with the Efficient Separations and Processing Crosscutting Program (EW4030000) and Westinghouse Savannah River Company.

Moyer, B. A., et. al. (1997, Oct. 15-17). Crown compounds as separation agents for environmental remediation from basic concepts to applications. Symposium on Molecular Sciences for the Environment, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory. Joint sponsorship with the Efficient Separations and Processing Cross-cutting Program (EW4030000) and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A., et. al. (1998, Jul. 27-30). Design and synthesis of the next generation of crown ethers for waste separations. DOE EMSP Scientific Workshop. Chicago, IL.

Moyer, B. A., et. al. (1999, Mar. 21-26). Alkaline-side CSEX process for Savannah River high-level waste. 217th American Chemical Society National Meeting. Anaheim, CA. Joint sponsorship with the Efficient Separations and Processing Crosscutting Program, Office of Science and Technology, Office of Environmental Management, U. S. Department of Energy.

Moyer, B. A., et. al. (2000, Jan. 26). Solvent extraction of fission products from alkaline nuclear waste. Invited presentation at Syracuse University, Syracuse, NY. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A., et. al. (2000, Mar. 26-31). Approaches to the remediation of alkaline high-level waste using solvent extraction. 219th National Meeting of the American Chemical Society, San Francisco, CA.

Moyer, B. A., et. al. (2000, Mar. 3). Fundamental research toward a process for nuclear-waste treatment: Cesium separation using calix-crown ethers. Invited presentation for the Department of Chemistry, Virginia Polytechnic Institute & State University, Blacksburg, VA. Joint sponsorship of the Efficient Separations and Processing Cross-cutting Program (EW4030000), Environmental Management Science Program (EW4090100), and the Office of Basic Energy Sciences (KC0302020), U. S. Department of Energy.

Moyer, B. A., Sachleben, R. A., & Alexandratos, S. D. (1999, Apr. 27-29). Ion exchange approach to the removal of ionic contaminants from groundwater. US DOE Subsurface Contamination Focus Area Mid-Year Review Meeting. Augusta, GA.

Moyer, B. A., Sachleben, R. A., Haverlock, T. J., & Alexandratos, S. D. (1999, Sept. 22). Ion exchange approach to the removal of ionic contaminants from groundwater. US DOE Oak Ridge Operations Environmental Management Science Program Workshop. Oak Ridge, TN.

Nicholas, J. B. & Hay, B. P. (1998, Jun. 17). A theoretical study of alkali cation complexes with tetramethoxycalix[4]arene. Northwest Regional American Chemical Society Meeting. Richland, WA.

Nicholas, J. B. & Hay, B. P. (1998, Jun. 6). A theoretical study of alkali cation complexes with tetramethoxycalix[4]arene. XXIII International Symposium on Macrocyclic Chemistry. Turtle Bay, Oahu, Hawaii.

Sachleben, R. A., et. al. (1999, Aug. 22-24). Calix[4]arene crown-6 ethers recent developments in enhanced cesium-selective extractants. 218th American Chemical Society National Meeting. New Orleans, LA.

Sachleben, R. A., et. al. (1999, Aug. 6). Recent developments in enhanced cesium-selective extractants calix[4]arene crown-6 ethers. DuPont Pharmaceuticals. N. Billerica, MA.

Sachleben, R. A., et. al. (1999, Mar. 21-26). Optimizing cesium-selective extraction by calix[4]arene crown ethers through ligand design. 217th American Chemical Society National Meeting. Anaheim, CA.

Sachleben, R. A., et. al. (1999, Sep. 19-23). Making the best even better enhancing the cesium selectivity of calixarene crown ethers through ligand design. Fifth International Conference on Calixarene Chemistry. Perth, Australia.

Yang, L., Dixon, D. A., & Hay, B. P. (1997, Jun. 6). MM3 calculations on alkali cation benzene complexes. International Conference on Structural and Mechanistic Organic Chemistry. Athens, GA.

Yang, L., Dixon, D. A., & Hay, B. P. (1997, Sep. 8). Molecular mechanics (MM3) calculations on calixarene complexes with alkali metal cations. The Importance of π -Cation Interactions. Inorganic Poster Session. 214th American Chemical Society Meeting. Las Vegas, NV.

Publication Type: Proceeding

Bond, A. H., Dietz, M. L., Huber, V. J., Herlinger, A. W., & Hay, B. P. (1999, Mar. 21). Diluent effects in synergistic solvent extraction by dicyclohexano-18-crown-6 and dialkylphosphoric acids. Abstr. Pap. Am. Chem. S. 217, U880-U880, Part 1.

Chiarizia, R., et. al. (1999, Jul. 11-16, in press). Synergistic effects in the extraction of metal ions by mixtures of dialkylphosphoric acids and substituted crown ethers. Proceedings of the International Solvent Extraction Conference, Barcelona, Spain.

Delmau, L. H., et. al. (2000). Benzyl phenol derivatives: Extraction properties of calixarene fragments. Lumetta, G. J., Rogers, R. D., & Gopalan, A. S. (Eds.). Calixarene Molecules for Separations. ACS Symposium Series, American Chemical Society, Washington, D. C. 757, 86-106.

Hay, B. P. (1999). A molecular mechanics method for predicting the influence of ligand structure on metal ion binding affinity. Bond, A. H., Dietz, M. L., & Rogers, R. D. (Eds.). Metal Ion Separation and Preconcentration: Progress and Opportunities. ACS Symposium Series 716, American Chemical Society, Washington, DC. 102-113.

Publication Type: Theses/Dissertations

Stine, C. L. (2000). Design and synthesis of the next generation of crown ethers for waste separations. Ph. D. dissertation, University of Tennessee, Knoxville, TN.

Project: 73824 (Renewal of Project No. 59982)

Title: Reactivity of Peroxynitrite: Implications for Hanford Waste Management and Remediation

PI: Dr. Sergei V. Lymar

Institution: Brookhaven National Laboratory

Publication Type: Journal

Coddington, J. W., Hurst, J. K., & Lymar, S. V. (1999). Hydroxyl radical formation during peroxynitrous acid decomposition. *J. Am. Chem. Soc.* 121, 2438-2443.

Coddington, J. W., Wherland, S., & Hurst J. K. (1999). Radical intermediates in peroxynitrite reactions. *Nitric Oxide.* 3, 37.

Czapski, G., Lymar, S. V., & Schwarz, H. A. (1999). Acidity of the carbonate radical. *J. Phys. Chem. A.* 103, 3447-3450.

Gerasimov, O. V. & Lymar, S. V. (1999). Pathways of decomposition and one-electron oxidation by peroxynitrous acid. *Nitric Oxide.* 3, 7.

Gerasimov, O. V. & Lymar, S. V. (1999, Sep. 20). The yield of hydroxyl radical from the decomposition of peroxynitrous acid. *Inorg. Chem.* 38(19), 4317-4321.

Goldstein, S., Saha, A., Lymar, S. V., & Czapski, G. (1998). Oxidation of peroxynitrite by inorganic radicals: A pulse radiolysis study. *J. Am. Chem. Soc.* 120, 5549-5554.

Lymar, S. V. & Hurst, J. K. (1998). ACO₂-catalyzed one-electron oxidations by peroxynitrite: Properties of the reactive intermediate. *Inorganic Chemistry.* 37, 294-301.

Lyman, S. V. & Hurst, J. K. (1998). Radical nature of peroxyxynitrite reactivity. *Chem. Res. Toxicol.* 11, 714-715.

Project: 74019 (Renewal of Project No. 54864)

Title: Supramolecular Chemistry of Selective Anion Recognition for Anions of Environmental Relevance

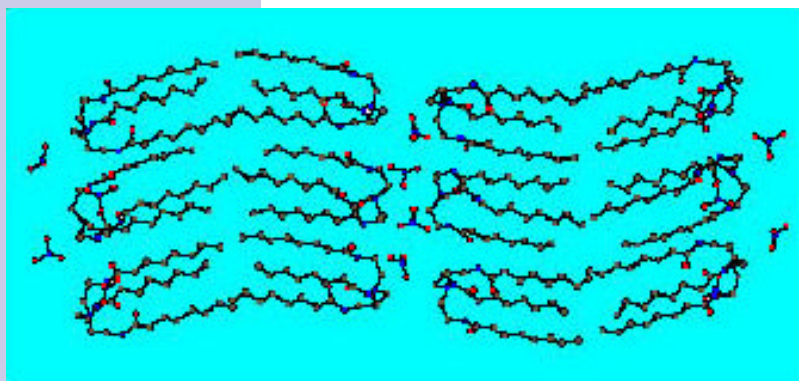
PI: Dr. Kristin Bowman-James

Institution: University of Kansas

Publication Type: Journal

Aguilar, J. A., et. al. (2000, in press). Fluoride ion receptors: A comparison of a polyammonium monocycle versus its bicyclic corollary. *Supramolec. Chem.*

Clifford, T., Mason, S., Llinares, J. M., & Bowman-James, K. (2000). Snapshots of fluoride binding in an Azacryptand. *J. Am. Chem. Soc.* 122, 1814-1815.



Contaminant Binding Science - The crystal structure of one of a tripodal lipophilic amide with nitrate ion, illustrated above, was developed for a University of Kansas project, which uses a combination of anion and cation complexing agents to extract cesium nitrate. [see Project #74019, renewal of #54864]

Danby, A., Seib, L., Alcock, N. W., & Bowman-James, K. (2000). Novel structural determination of a bilayer network formed by a tripodal lipophilic amide in the presence of anions. *Chem. Commun.* 39, 1371-1375.

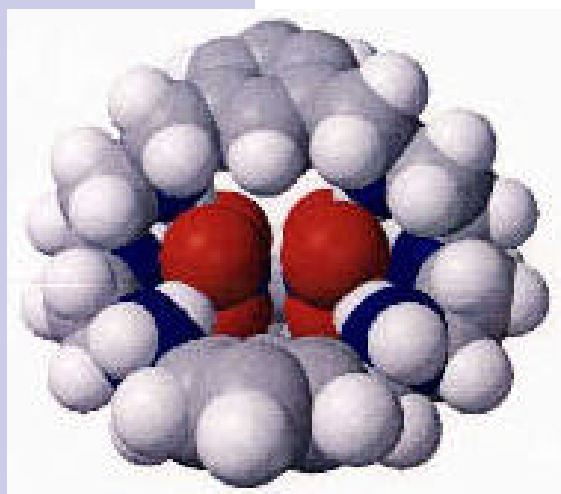
Gerasimchuk, O. A., et. al. (2000, Apr. 3). Binding of phosphate with a simple hexaaza polyammonium macrocycle. *Inorg. Chem.* 39(7), 1371-1375.

Hossain, M. A., Llinares, J. M., Powell, D., & Bowman-James, K. (2001, in press). Multiple hydrogen bond stabilization of a sandwich complex of sulfate between two macrocyclic tetraamides. *Inorg. Chem.*

Kavallieratos, K., et. al. (2000). Tris(2-aminoethyl)amine (tren) triamide derivatives enhance CsNO₃ extraction in 1,2-dichloroethane via a dual-host strategy. *Anal. Chem.* 72, 5258-6264.

Mason, S., Clifford, T., Seib, L., Kuczera, K., & Bowman-James, K. (1998). Unusual encapsulation of two nitrates in a single bicyclic cage. *J. Am. Chem. Soc.* 120, 8899-8900.

Qian, Q., Wilson, G. S., Bowman-James, K., & Girault, H. H. (2001). Microities detection of NO₃⁻ by facilitated k⁺ transfer. *Anal. Chem.* 73, 497-503.



Nitrate inclusion complex with a polyammonium receptor. [see Project #74019, renewal of #54864]

Wiórkiewicz-Kuczera, et. al. (1999). Solid state to solution: Crystal structure and molecular dynamics simulations of a polyammonium nitrate host, *New J. Chem.* 23, 1007-1013.

Publication Type: Other

Bianchi, A., Bowman-James, K., & García-España, E. (Eds.). (1997), *Supramolecular Chemistry of Anions*, Wiley-VCH. New York, NY. 461.

Wiórkiewicz-Kuczera, J. & Bowman-James, K. (1997). Anion Binding Receptors: Theoretical Studies. Bianchi, A., Bowman-James, K., & García-España, E. (Eds.), *Supramolecular Chemistry of Anions*. Wiley-VCH, New York, NY. 335-354.

Publication Type: Paper

Bowman-James, K. & Mason, S. (1998, Aug.). *Supramolecular chemistry of anions*. 216th National Meeting of the American Chemical Society, Boston, MA.

Bowman-James, K. (1999, Jul. 18-23). *Supramolecular chemistry of anions and macrocycles*. Plenary Lecture at the XXIV International Symposium on Macrocyclic Chemistry, Bellaterra (Barcelona), Spain.

Bowman-James, K. (2000, Jul. 2-7). *Exploration in anion coordination chemistry*. Symposium Lecture at the XXV International Symposium on Macrocyclic Chemistry, Saint Andrews, Scotland.

Kavallieratos, K., et. al. (1999, Mar.). *New anion receptors and their role in solvent extraction*. 217th National Meeting of the American Chemical Society, Anaheim, CA.

Publication Type: Press release

Moyer, B. A. (1998, Sep. 7). *Two nitrates in a cage*. C&E News concentrate. 30.

Project: 81883

Title: Mechanisms and Kinetics of Organic Aging and Characterization of Intermediates in High-Level Waste

PI: Dr. Donald M. Camaioni

Institution: Pacific Northwest National Laboratory

Publication Type: Journal

Cook, A. R., et. al. (2001, in press). *Reducing radicals in nitrate solutions. The NO₃ system revisited*. *J. Phys. Chem. A*.

Fessenden, R. D., Meisel, D., & Camaioni, D. M. (2000). *Addition of oxide radical ions (O) to nitrite and oxide ions (O₂) to nitrogen dioxide*. *J. Am. Chem. Soc.* 122, 3773-3774.

Publication Type: Poster

Camaioni, D. M., Dupuis, M., & Franz, J. A. (2000, Jun. 29). Theoretical characterization of organic radicals in solution. Gomberg 2000 (8th International Symposium on Organic Free Radicals). Ann Arbor, MI.

Publication Type: Presentation

Autrey, S. T. (1999, Apr. 30). Nitrosyl transfer reactions are not catalyzed by Al(OH)₄. Notre Dame Radiation Laboratory and Pacific Northwest National Laboratory EEMSP Coordination Meeting and Technical exchange. Notre Dame, IN.

Camaioni, D. M. (1998, Nov. 17). Mechanisms and kinetics of organic aging in high level wastes. EMSP/Tanks Focus Area Workshop. Richland, WA.

Camaioni, D. M. (1998, Oct. 29). Mechanisms and kinetics of the degradation of organic complexants in nuclear waste. Chemistry Seminar, Notre Dame Radiation Laboratory. Notre Dame, IN.

Camaioni, D. M. (1999, Aug. 22-26). Thermochemical kinetic analysis of thermal pathways for oxidation of organic complexants in high level wastes. First Accomplishments of the Environmental Management Science Program. Annual Meeting of the American Chemical Society. New Orleans, LA.

Camaioni, D. M., Orlando, T. M., & Meisel, D. (2000, Apr. 25-27). Radiolytic and thermal processes in homogenous and heterogenous high level waste. EMSP National Workshop. Atlanta, GA.

Dupuis, M. (1999, Aug.). Electronic structure and reactivity in the condensed phase. Physical Chemistry Colloquium. Department of Chemistry. University of Notre Dame. South Bend, IN.

Dupuis, M. (1999, Nov.). Theoretical characterization of electronic structure and reactivity in the condensed phase. Department of Chemistry. University of Alberta. Edmonton, Alberta, Canada.

Dupuis, M. (2000, Mar.). Electronic structure and reactivity in the condensed phase: Computational studies. Physical Chemistry Seminar. Department of Chemistry. University of Washington. Seattle, WA.

Dupuis, M. (2001, Oct.). Recent research on electronic structure and reactivity in the aqueous phase. University of Tokyo. Tokyo, Japan.

Dupuis, M. (2001, Oct.). Recent research on electronic structure and reactivity in the aqueous phase. University of Kyoto. Kyoto, Japan.

Publication Type: Proceeding

Babad, H. & Camaioni, D. M. (2000, Feb. 27 - Mar. 2). The aging of organic chemicals in Hanford high-level wastes. Proceedings of the Waste Management 2000 Conference. Tucson, AZ.

Camaioni, D. M. & Autrey, S. T. (2000). Thermochemical kinetic analysis of mechanism for thermal oxidation of organic complexants in high level waste. In Eller, P. G. & Heineman, W. R. (Eds.). Nuclear Site Remediation on First Accomplishments of the Environmental Management Program. ACS Symposium Ser. 778. American Chemical Society. Washington, D. C. 21, 342-361.

Dupuis, M. (2000, Mar.). Electronic structure and reactivity in the condensed phase: Computational studies. Symposium on "Potential Energy Surfaces: From Polyatomics to Macromolecules." 219th American Chemical Society National Meeting. San Francisco, CA.

Meisel, D., Camaioni, D. M., & Orlando, T. M. (2000). Radiation and chemistry in nuclear waste: The NO_x system and organic aging. In Eller, P. G. & Heineman, W. R. (Eds.). Nuclear Site Remediation on First Accomplishments of the Environmental Management Program. ACS Symposium Ser. 778. American Chemical Society. Washington, D. C. 21, 342-361.

Project: 81912 (Renewal of Project No. 65409)

Title: Electroactive Materials for Anion Separation – Technetium from Nitrate

PI: Timothy L. Hubler

Institution: Pacific Northwest National
Laboratory

Publication Type: Presentation

Gronda, A. M. & Smyrl, W. H. (1999, Oct. 17-22). High capacity electroactive polymers for radioactive waste removal. Abstract at the 196th Electrochemical Society Meeting. Honolulu, HI.

Hubler, T. L., Anderson, G. M., Sukamto, J. H., Lilga, M. A., & Rassat, S. D. (1999, Aug. 22). Polyvinylferrocene (PVF) polymers as electroactive ion-exchange materials for separation of pertechnetate ion from high nitrate ion containing wastes: Issues and synthetic strategies. Abstr. Pap. Am. Chem. S. 218, U1050-U1050, Part 1.