

Publications

Publications by EMSL staff members and from users where the publication resulted from research carried out at EMSL are listed below.

Adkins JN, HM Mottaz, AD Norbeck, JK Gustin, J Rue, T Clauss, SO Purvine, KD Rodland, F Heffron, and RD Smith. 2006. "Analysis of the *Salmonella typhimurium* Proteome through Environmental Response toward Infectious Conditions." *Molecular & Cellular Proteomics. MCP* 5(8):1450-1461. doi:10.1074/mcp.M600139-MCP200

Ainsworth CC, JM Zachara, K Wagnon, S McKinley, C Liu, SC Smith, HT Schaef, and PL Gassman. 2005. "Impact of Highly Basic Solutions on Sorption of Cs⁺ to Subsurface Sediments from the Hanford Site, USA." *Geochimica et Cosmochimica Acta* 69(20):4787-4800.

Alam TM, BR Cherry, KR Minard, and M Celina. 2005. "Relaxation Nuclear Magnetic Resonance Imaging Investigation of Heterogeneous Aging in a Hydroxy-Terminated Polybutadiene-Based Elastomer." *Macromolecules* 38(26):10694-10701.

Alvarez J, JH Futrell, and J Laskin. 2006. "Soft-Landing of Peptides onto Self-Assembled Monolayer Surfaces." *Journal of Physical Chemistry A* 110(4):1678-1687.

Antony J, Y Qiang, DR Baer, and C Wang. 2006. "Synthesis and Characterization of Stable Iron–Iron Oxide Core–Shell Nanoclusters for Environmental Applications." *Journal of Nanoscience and Nanotechnology* 6(2):568-572.

Apra E, R Ferrando, and A Fortunelli. 2006. "Density-Functional Global Optimization of Gold Nanoclusters." *Physical Review B. Condensed Matter* 73(20):205414 -1 - 205414-5.

Armstrong RC, GK Kumfert, LC McInnes, SG Parker, BA Allan, S Matt, TG Epperly, and TL Dahlgren. 2006. "The CCa Component Model for High-Performance Scientific Computing." *Concurrency and Computation. Practice & Experience* 18(2):215-229.

Asplund MC, AM Johnson, and JA Jakeman. 2006. "Time-Resolved Infrared Dynamics of C-F Bond Activation by a Tungsten Metal-Carbonyl." *Journal of Physical Chemistry B* 110(1):20-24.

Auer AA, G Baumgartner, DE Bernholdt, A Bibireata, V Choppella, D Cociorva, X Gao, R Harrison, S Krishnamoorthy, S Krishnan, CC Lam, Q Lu, M Nooijen, R Pitzer, J Ramanujam, P Sadayappan, and A Sibiryakov. 2006. "Automatic Code Generation for Many-Body Electronic Structure Methods: The Tensor Contraction Engine ‡." *Molecular Physics* 104(2):211-228.

Bagus P, C Woll, and ES Ilton. 2006. "A Definitive Analysis of the Rydberg and Valence Anti-Bonding Character of States in the O K-edge of H₂O." *Chemical Physics Letters* 428(1-3):207-212. doi:10.1016/j.cplett.2006.07.030

Bai J, LF Cui, J Wang, S Yoo, X Li, J Jellinek, C Koehler, T Frauenheim, LS Wang, and XC Zeng. 2006. "Structural Evolution of Anionic Silicon Clusters Si_n (20 ≤ n ≤ 45)." *Journal of Physical Chemistry A* 110(3):908-912.

Barlow SE, and MD Tinkle. 2006. "The Ion Cyclotron Resonance Frequency of Short, Single-Species Plasmas in Penning Traps." *Journal of Applied Physics* 99(1):013306 (pages 1-8).

Bayard E, S Hamel, and A Rochefort. 2006. "Hydrogen Bonding and Pi-Stacking in Highly Organized Arenes-Based Molecular Wire." *Organic Electronics* 7(3):144-154.

Beck KM, M Henyk, CM Wang, PE Trevisanutto, PV Sushko, WP Hess, and AL Shluger. 2006. "Site-Specific Laser Modification of MgO Nanoclusters: Towards Atomic-Scale Surface Structuring." *Physical Review B. Chemical Matter and Materials Physics* 74(4): Art. No. 045404.

Berben LA, FC Mary, NR Crawford, and J Long. 2006. "Angle-Dependent Electronic Effects in 4,4'-Bipyridine-Bridged Ru₃ Triangle and Ru₄ Square Complexes." *Inorganic Chemistry* 45(16):6378-6386.

Bernholdt DE, BA Allan, RC Armstrong, F Bertrand, K Chiu, TL Dahlgren, K Damevski, WR Elwasif, TG Epperly, M Govindaraju, DS Katz, JA Kohl, M Krishnan, GK Kumfert, J Larson, S Lefantzi, MJ Lewis, AD Malony, LC McInnes, J Nieplocha, B Norris, SG Parker, J Ray, S Shende, TL Windus, and S Zhou. 2006. "A Component Architecture for High-Performance Scientific Computing." *International Journal of High-Performance Computing Applications* 20(2):163-202.

Bickmore BR, KM Rosso, CJ Tadanier, EJ Bylaska, and D Doud. 2006. "Bond-Valence Methods for pKa Prediction. II. Bond-Valence, Electrostatic, Molecular Geometry, and Solvation Effects." *Geochimica et Cosmochimica Acta* 70(16):4057-4071.

Blake TA and SS Xantheas. 2006. "Structure, Vibrational Spectra, and Ring Puckering Barrier of Cyclobutane." *Journal of Physical Chemistry A* 110(35):10487-10494.

Boily J, J Szanyi, and AR Felmy. 2006. "A Combined FTIR and TPD Study on the Bulk and Surface Dehydroxylation and Decarbonation of Synthetic Goethite." *Geochimica et Cosmochimica Acta* 70(14):3613-3624.

Bondarchuk O, X Huang, J Kim, BD Kay, LS Wang, JM White, and Z Dohnalek. 2006. "Formation of Monodisperse (WO₃)₃ Clusters on TiO₂(110)." *Angewandte Chemie-International Edition* 45(29):4786-4789.

Bowers GM, AS Lipton, and KT Mueller. 2006. "High-Field QCPMG NMR of Strontium Nuclei in Natural Minerals." *Solid State Nuclear Magnetic Resonance* 29(1-3):95-103.

Bowers GM, R Ravella, S Komarneni, and KT Mueller. 2006. "NMR Study of Strontium Binding by a Micaceous Mineral." *Journal of Physical Chemistry B* 110(14):7159-7164.

- Brim H, JP Osborne, HM Kostandarithis, JK Fredrickson, LP Wackett, and MJ Daly. 2006. "Deinococcus radiodurans Engineered for Complete Toluene Degradation Facilitates Cr(VI) Reduction." *Microbiology* 152(8):2469-2477.
- Bryantsev V, and BP Hay. 2006. "Conformational Preferences and Internal Rotation in Alkyl- and Phenyl-Substituted Thiourea Derivatives." *Journal of Physical Chemistry A* 110(14):4678-4688.
- Brzovic PS, J O'Keeffe, DE Christensen, DW Hoyt, and RE Klevit. 2006. "A UbCH5/Ubiquitin Noncovalent Complex is Required for Processive BRCA1-Directed Ubiquitination." *Molecular Cell* 12(6):873-880.
- Buchko GW, CY Kim, TC Terwilliger, and MA Kennedy. 2006. "Solution Structure of the Conserved Hypothetical Protein Rv2302 from the Bacterium *Mycobacterium tuberculosis*." *Journal of Bacteriology* 188(16):5993-6001.
- Bulusu S, X Li, LS Wang, and X Zeng. 2006. "Evidence of Hollow Golden Cages." *Proceedings of the National Academy of Sciences* 103(22):8326-8330.
- Bylaska EJ, K Tsemekhman, and F Gao. 2006. "New Development of Self-Interaction Corrected DFT for Extended Systems Applied to the Calculation of Native Defects in 3C-SiC." *Physica Scripta* T124:86-90.
- Callister SJ, RC Barry, JN Adkins, ET Johnson, WJ Qian, BJM Webb-Robertson, RD Smith, and MS Lipton. 2006. "Normalization Approaches for Removing Systematic Biases Associated with Mass Spectrometry and Label-Free Proteomics." *Journal of Proteome Research* 5(2):277-286.
- Callister SJ, M Dominguez, CD Nicora, X Zeng, C Tavano, S Kaplan, T Donohue, RD Smith, and MS Lipton. 2006. "Application of the Accurate Mass and Time Tag Approach to the Proteome Analysis of Sub-Cellular Fractions Obtained from *Rhodobacter sphaeroides* 2.4.1 Aerobic and Photosynthetic Cell Cultures." *Journal of Proteome Research* 5(8):1940-1947.
- Cape JL, MK Bowman, and DM Kramer. 2006. "Understanding the Cytochrome bc Complexes by What They Don't Do. The Q-Cycle at 30." *Trends in Plant Science* 11(1):46-55.
- Carissan Y, F Bessac, F Alary, JL Heully, and R Poteau. 2006. "What Can We Do with an Effective Group Potential?" *International Journal of Quantum Chemistry* 106(3):727-733.
- Chekmenev EY, SM Jones, Y Nikolayeva, B Vollmar, TJ Wagner, PL Gorkov, WW Brey, MN Manion, KC Daugherty, and M Cotten. 2006. "High-Field NMR Studies of Molecular Recognition and Structure-Function Relationships in Antimicrobial Piscidins at the Water-Lipid Bilayer Interface." *Journal of the American Chemical Society* 128(16):5308-5309.

Chen W, G Huang, HB Lu, DE McCready, AG Joly, and JO Bovin. 2006. "Utilizing Nanofabrication to Construct Strong, Luminescent Materials." *Nanotechnology* 17(10):2595-2601.

Chen W, J Zhang, SL Westcott, AG Joly, JO Malm, and JO Bovin. 2006. "The Origin of X-Ray Luminescence from CdTe Nanoparticles in CdTe/BaFBr:Eu²⁺ Nanocomposite Phosphors." *Journal of Applied Physics* 99(3):034302.

Cho H, AR Felmy, R Craciun, JP Keenum, N Shah, and DA Dixon. 2006. "Solution State Structure Determination of Silicate Oligomers by ²⁹Si NMR Spectroscopy and Molecular Modeling." *Journal of the American Chemical Society* 128(7):2324-2335.

Craig NC, MC Moore, AK Patchen, and RL Sams. 2006. "Analysis of Rotational Structure in the High-Resolution Infrared Spectrum and Assignment of Vibrational Fundamentals of Butadiene-2,3-C-13(2)." *Journal of Molecular Spectroscopy* 235(2):181-189.

Cui LF, X Huang, LM Wang, J Li, and LS Wang. 2006. "Pb-12(2-): Plumbaspherene." *Journal of Physical Chemistry A* 110(34):10169-10172.

Cui L, X Huang, LM Wang, DY Zubarev, AI Boldyrev, J Li, and LS Wang. 2006. "Sn₁₂²⁻: Stannaspherene." *Journal of the American Chemical Society* 128:8390-8391.

Cui LF, X Li, and LS Wang. 2006. "Photoelectron Spectroscopy of Al_nD₂⁻ (n=3-15): Observation of Chemisorption and Physisorption of Dideuterium on Aluminum Cluster Anions." *Journal of Chemical Physics* 124(5):054308.

Cui X, MH Engelhard, and Y Lin. 2006. "Preparation, Characterization and Anion Exchange Properties of Polypyrrole/Carbon Nanotube Nanocomposite." *Journal of Nanoscience and Nanotechnology* 6(2):547-553.

Custelcean R., BA Moyer, VS Bryantsev, and BP Hay. 2006. "Anion Coordination in Metal-Organic Frameworks Functionalized with Urea Hydrogen-Bonding Groups." *Crystal Growth and Design* 6(2):555-563.

Devanathan R, LR Corrales, WJ Weber, A Chartier, and C Meis. 2006. "Atomistic Simulation of Collision Cascades in Zircon." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 250(1-2):46-49.
doi:10.1016/j.nimb.2006.04.109

Diamond DL, S Proll, JM Jacobs, EY Chan, DG Camp, II, RD Smith, and MG Katze. 2006. "HepatoProteomics: Applying Proteomic Technologies to the Study of Liver Function and Disease." *Hepatology* 44(2):299-308.

Ding YR, KK Hixson, CS Giometti, A Stanley, A Esteve-Nunez, T Khare, S Tollaksen, W Zhu, JN Adkins, MS Lipton, RD Smith, T Mester, and DR Lovley. 2006. "The Proteome of Dissimilatory Metal-Reducing Microorganism *Geobacter sulfurreducens* under Various Growth Conditions." *Biochimica et Biophysica Acta--Proteins and Proteomics*. 1764(7):1198-1206.

Disselkamp RS, RG Tonkyn, YH Chin, and CHF Peden. 2006. "Developing Multiple-Site Kinetic Models in Catalysis Simulation: A Case Study of O₂+2NO <-> 2NO₂ Oxidation-Reduction Chemistry on Pt(100) Catalyst Crystal Facets." *Journal of Catalysis* 238(1):1-5.

Dixon DA, and AJ Arduengo III. 2006. "Accurate Heats of Formation of the "Arduengo-Type" Carbene and Various Adducts Including H₂ from *ab initio* Molecular Orbital Theory." *Journal of Physical Chemistry A* 110(5):1968-1974.

Dixon DA, JS Francisco, and Y Alexeev. 2006. "Thermochemical Properties of H_xNO Molecules and Ions from *ab initio* Electronic Structure Theory." *Journal of Physical Chemistry A* 110(1):185-191.

Dobson R, MH Schroth, M Oostrom, and J Zeyer. 2006. "Determination of NAPL-Water Interfacial Areas in Well-Characterized Porous Media." *Environmental Science and Technology* 40(3):815-822.

Dohnalek Z, J Kim, O Bondarchuk, JM White, and BD Kay. 2006. "Physisorption of N₂, O₂, and CO on Fully Oxidized TiO₂(110)." *Journal of Physical Chemistry B* 110(12):6229-6235.

Du S, J Francisco, GK Schenter, TD Iordanov, BC Garrett, M Dupuis, and J Li. 2006. "The OH Radical-H₂O Molecular Interaction Potential." *Journal of Chemical Physics* 124:224318-1-224318-15.

El-Shafey A, N Tolic, MM Young, K Sale, RD Smith, and V Kery. 2006. "Zero-Length" Cross-Linking in Solid State as an Approach for Analysis of Protein-Protein Interactions." *Protein Science* 15(3):429-440.

Elliott BM, E Koyle, AI Boldyrev, XB Wang, and LS Wang. 2005. "MX₃ Superhalogens (M = Be, Mg, Ca; X = Cl, Br): A Photoelectron Spectroscopic and *ab initio* Theoretical Study." *Journal of Physical Chemistry A* 109(50):11560-11567.

Elliott DC. 2006. "Catalytic Hydrogenation of Bio-Oil for Chemicals and Fuels." *PyNe* 2006(1):5.

Elliott DC, GG Neuenschwander, TR Hart, J Hu, AE Solana, and C Cao. 2006. "Hydrogenation of Bio-Oil for Chemicals and Fuels Production." In *Science in Thermal and Chemical Biomass Conversion*, Vol. 2, AV Bridgwater and DGB Boocock, eds., pp. 1536-1546, CPL Press, Newbury, Berkshire, Great Britain.

Fan P and S Hirata. 2006. "Active-Space Coupled-Cluster Methods through Connected Quadruple Excitations." *Journal of Chemical Physics* 124:104108-104117.

Fang R, DA Elias, ME Monroe, Y Shen, M McIntosh, P Wang, CD Goddard, SJ Callister, RJ Moore, YA Gorby, JN Adkins, JK Fredrickson, MS Lipton, and RD Smith. 2006. "Differential Label-Free Quantitative Proteomic Analysis of *Shewanella oneidensis* Cultured under Aerobic and Suboxic Conditions by Accurate Mass and Time Tag Approach." *Molecular & Cellular Proteomics* 5:714-725.

- Feller D, KA Peterson, and TD Crawford. 2006. "Sources of Error in Electronic Structure Calculations on Small Chemical Systems." *Journal of Chemical Physics* 124(5):054107.
- Felmy AR, HM Cho, DA Dixon, Y Xia, NJ Hess, and Z Wang. 2006. "The Aqueous Complexation of Thorium with Citrate under Neutral to Basic Conditions." *Radiochimica Acta* 94(4):205-212.
- Felmy AR, EJ Bylaska, DA Dixon, M Dupuis, JW Halley, R Kawai, KM Rosso, JR Rustad, PE Smith, T Straatsma, GA Voth, JH Weare, and DA Yuen. 2006. *Computational Studies in Molecular Geochemistry and Biogeochemistry*. PNNL-15462, Pacific Northwest National Laboratory, Richland, Washington.
- Fernandez FM, VH Wysocki, JH Futrell, and J Laskin. 2006. "Protein Identification via Surface-Induced Dissociation in an FT-ICR Mass Spectrometer and a Patchwork Sequencing Approach." *Journal of the American Society for Mass Spectrometry* 17(5):700-709.
- Fir B, M Whalen, H Mercier, DA Dixon, and GJ Schrobilgen. 2006. "Syntheses of $[F_5TeNH_3][AsF_6]$, $[F_5TeN(H)Xe][AsF_6]$, and F_5TeNF_2 and Characterization by Multi-NMR and Raman Spectroscopy and by Electronic Structure Calculations: The X-ray Crystal Structures of α - and β - F_5TeNH_2 , $[F_5TeNH_3][AsF_6]$, and $[F_5TeN(H)Xe][AsF_6]$." *Inorganic Chemistry* 45(5):1978-1996.
- Flaud JM, WJ Lafferty, RL Sams, and SW Sharpe. 2006. "High Resolution Spectroscopy of $(H_2CO)-C-12-O-16$ in the 1.9 to 2.56 μm Spectral Range." *Molecular Physics* 102(12):1891-1903.
- Forgeron MAM and RE Wasylyshen. 2006. "A Solid-State 95Mo NMR and Computational Investigation of Dodecahedral and Square Antiprismatic Octacyanomolybdate(IV) Anions: Is the Point-Charge Approximation an Accurate Probe of Local Symmetry?" *Journal of the American Chemical Society* 128(24):7817-7827.
- Fox PM, JA Davis, and JM Zachara. 2006. "The Effect of Calcium on Aqueous Uranium (VI) Speciation and Adsorption to Ferrihydrite and Quartz." *Geochimica et Cosmochimica Acta* 70(6):1379-1387.
- Francisco JS, SM Kathmann, GK Schenter, LX Dang, SS Xantheas, BC Garrett, S Du, DA Dixon, R Bianco, S Wang, JT Hynes, A Morita, and KA Peterson. 2006. *A Computational Approach to Understanding Aerosol Formation and Oxidant Chemistry in the Troposphere*. PNNL-15772, Pacific Northwest National Laboratory, Richland, Washington.
- Fu YJ, J Laskin, and LS Wang. 2006. "Collision-Induced Dissociation of [4Fe-4S] Cubane Cluster Complexes: $[Fe_4S_4Cl_{4-x}(SC_2H_5)(x)](2-/1-)$ ($x=0-4$).". *International Journal of Mass Spectrometry* 255:102-110.
- Gallagher NB, TA Blake, and PL Gassman. 2005. "Application of Extended Inverse Scatter Correction to Mid-Infrared Reflectance Spectra of Soil." *Journal of Chemometrics* 19(5-7):271-281.

Gallagher NB, TA Blake, PL Gassman, JM Shaver, and W Windig. 2006. "Multivariate Curve Resolution Applied to Infrared Reflection Measurements of Soil Contaminated with an Organophosphorus Analyte." *Applied Spectroscopy* 60(7):713-722.

Gao F, R Devanathan, T Oda, and WJ Weber. 2006. "Development of Partial-Charge Potential for GaN." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 250(1-2):50-53.

Gao F, R Devanathan, Y Zhang, M Posselt, and WJ Weber. 2006. "Atomic-Level Simulation of Epitaxial Recrystallization and Phase Transformation in SiC." *Journal of Materials Research* 21(6):1420-1426.

Gao F, Y Zhang, M Posselt, and WJ Weber. 2006. "Atomic-Level Simulations of Epitaxial Recrystallization and Amorphous-to-Crystalline Transition in 4H-SiC." *Physical Review B. Condensed Matter and Materials Physics* 74(10): Art. No. 104108, 1-9.

Gelb LD, and TN Carnahan. 2006. "Isothermal-Isobaric Monte Carlo Simulations of Liquid Lithium Using Density Functional Theory." *Chemical Physics Letters* 417(4-6):283-287.

Gorby YA, S Yanina, JS Mclean, KM Rosso, DM Moyles, A Dohnalkova, TJ Beveridge, I Chang, BH Kim, KS Kim, DE Culley, SB Reed, MF Romine, D Saffarini, EA Hill, L Shi, DA Elias, DW Kennedy, GE Pinchuk, K Watanabe, S Ishii, B Logan, KH Nealson, and JK Fredrickson. 2006. "Electrically Conductive Bacterial Nanowires Produced by *Shewanella oneidensis* Strain MR-1 and Other Microorganisms." *Proceedings of the National Academy of Sciences of the United States of America* 103(30):11358-11363.

Groenewold GS, AK Gianotto, KC Cossel, MJ Van Stipdonk, DT Moore, N Polfer, J Oomens, WA De Jong, and L Visscher. 2006. "Vibrational Spectroscopy of Mass-Selected $[UO_2(\text{ligand})n]^{2+}$ Complexes in the Gas Phase: Comparison with Theory." *Journal of the American Chemical Society* 128:4802-4813.

Gu Z, L Du, JH Edgar, EA Payzant, HM Meyer, L Walker, R Liu, and MH Engelhard. 2006. "Aluminum Nitride-Silicon Carbide Alloy Crystals Grown on SiC Substrates by Sublimation." *MRS Internet Journal of Nitride Semiconductor Research* 10(5)

Gu Z, JH Edgar, CM Wang, and D Coffey. 2006. "Thermal Oxidation of Aluminum Nitride Powder." *Journal of the American Ceramic Society* 89(7):2167–2171.

Gun'ko VM, VV Turov, V Barvinchenko, VM Bogatyrev, AV Turov, OV Shulga, O Stebelska, V Pokrovsky, R Leboda, V Sukretny, Y Nychiporuk, Y Gornikov, B Chuikov, and Y Ptushinskii. 2006. "Characteristics of Interfacial Water at Nanosilica Surface with Adsorbed 1,3,5-Trihydroxybenzene Over Wide Temperature Range." *Colloids and Surfaces A, Physicochemical and Engineering Aspects* 278:106-122.

Haynes PD, C Skylaris, AA Mostofi, and M Payne. 2006. "Elimination of Basis Set Superposition Error in Linear-Scaling Density-Functional Calculations with Local Orbitals Optimised *In Situ*." *Chemical Physics Letters* 422(4-6):345-349.

Herrera JE, J K Wak, J Hu, Y Wang, CH Peden, J Macht, and E Iglesia. 2006. "Synthesis, Characterization, and Catalytic Function of Novel Highly Dispersed Tungsten Oxide Catalysts on Mesoporous Silica." *Journal of Catalysis* 239(1):200-211.

Hu J, RA Wind, and DN Rommereim. 2006. "H-1 Relaxation Times of Metabolites in Biological Samples Obtained with Nondestructive Ex-Vivo Slow-MAS NMR ." *Magnetic Resonance in Chemistry* 44(3):269-275. doi:10.1002/mrc.1764

Huang X., HJ Zhai, J Li, and LS Wang. 2006. "On the Structure and Chemical Bonding of Tri-Tungsten Oxide Clusters $W_3O_n^-$ and W_3O_n ($n = 7-10$): W_3O_8 as a Potential Molecular Model for O-Deficient Defect Sites in Tungsten Oxides." *Journal of Physical Chemistry A* 110(1):85-92.

Huang X, HJ Zhai, T Waters, J Li, and LS Wang. 2006. "Experimental and Theoretical Characterization of Superoxide Complexes [$W_2O_6(O_2^-)$] and [$W_3O_9(O_2^-)$]: Models for the Interaction of O_2 with Reduced W Sites on Tungsten Oxide Surfaces." *Angewandte Chemie International Edition* 45(4):657-660.

Hughes M, D Nielsen, E Rosenberg, R Gobetto, A Viale, SD Burton, and JJ Ford. 2006. "Structural Investigations of Silica Polyamine Composites: Surface Coverage, Metal Ion Coordination, and Ligand Modification." *Industrial and Engineering Chemistry Research* 45(19):6538-6547.

Ibrahim YM, K Tang, AV Tolmachev, AA Shvartsburg, and RD Smith. 2006. "Improving Mass Spectrometer Sensitivity Using a High-Pressure Electrodynamic Ion Funnel Interface." *Journal of the American Society for Mass Spectrometry* 17(9):1299-1305.

Ilton ES, SM Heald, SC Smith, D Elbert, and C Liu. 2006. "Reduction of Uranyl in the Interlayer Region of Low Iron Micas under Anoxic and Aerobic Conditions." *Environmental Science & Technology* 40(16):5003-5009.

Jackson SM. 2006. "Allocation Management Solutions for High Performance Computing." In *Proceedings of the 2005 International Conference on Parallel and Distributed Processing Techniques and Applications* 1-3:10-16, CSREA Press, Athens, Greece.

Jiang W, V Shutthanandan, Y Zhang, S Thevuthasan, WJ Weber, and GJ Exarhos. 2006. "Hydrogen Behavior in Mg⁺-Implanted Graphite." *Journal of Materials Research* 21(4):811-815.

Jiang W, and WJ Weber. 2006. "Effect of Irradiation Temperature on Dynamic Recovery in Gallium Nitride." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 242(1-2):431-433.

Jiang W, Y Zhang, WJ Weber, J Lian, and RC Ewing. 2006. "Direct Evidence of N Aggregation and Diffusion in Au+ Irradiated GaN." *Applied Physics Letters* 89(2):021903-1—021903-3.

- Joensson CT, IA Maximov, HJ Whitlow, V Shuthananadan, LV Saraf, DE McCready, BW Arey, Y Zhang, and S Thevuthasan. 2006. "Synthesis and Characterization of Cobalt Silicide Films on Silicon." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 249(1-2):532–535.
- Johnson TJ, T Masiello, and SW Sharpe. 2006. "The Quantitative Infrared and NIR Spectrum of CH₂I₂ Vapor: Vibrational Assignments and Potential for Atmospheric Monitoring." *Atmospheric Chemistry and Physics* 6(9):2581-2591.
- Joly AG, M Henyk, KM Beck, PE Trevisanutto, PV Sushko, WP Hess, and AL Shluger. 2006. "Probing Electron Transfer Dynamics at MgO Surfaces by Mg-Atom Desorption." *Journal of Physical Chemistry B* 110(37):18093-18096.
- Joly AG, JR Williams, SA Chambers, G Xiong, WP Hess, and DM Laman. 2006. "Carrier Dynamics in α -Fe₂O₃(0001) Thin Films and Single Crystals Probed by Femtosecond Transient Absorptivity and Reflectivity." *Journal of Applied Physics* 99(5):053521.
- Kaspar TC, TC Droubay, V Shuthananadan, SM Heald, CM Wang, DE McCready, S Thevuthasan, JD Bryan, DR Gamelin, AJ Kellock, MF Toney, X Hong, C Ahn, and SA Chambers. 2006. "Ferromagnetism and Structure of Epitaxial Cr-doped Anatase TiO₂ Thin Films." *Physical Review. B, Condensed Matter and Materials Physics* 73(15):155327.
- Keske JC, W Lin, WC Pringle, SE Novick, TA Blake, and DF Plusquellec. 2006. "High-Resolution Studies of Tropolone in the S₀ and S₁ Electronic States: Isotope Driven Dynamics in the Zero-Point Energy Levels." *Journal of Chemical Physics* 124(7):074309.
- Kiebel GR, KJ Auberry, N Jaitly, DA Clark, ME Monroe, ES Peterson, N Tolic, GA Anderson, and RD Smith. 2006. "PRISM: A Data Management System for High-Throughput Proteomics." *Proteomics* 6(6):1783-1790.
- Kim D, J Szanyi, J Kwak, T Szailer, J Hanson, CM Wang, and CH Peden. 2006. "Effect of Barium Loading on the Desulfation of Pt-BaO/Al₂O₃ Studied by H₂ TPRX, TEM, Sulfur K-edge XANES, and *In Situ* TR-XRD." *Journal of Physical Chemistry B* 110(21):10441-10448.
- Kim J, H Jia, C Lee, S Chung, J Kwak, Y Shin, A Dohnalkova, B Kim, P Wang, and JW Grate. 2006. "Single Enzyme Nanoparticles in Nanoporous Silica: A Hierarchical Approach to Enzyme Stabilization and Immobilization." *Enzyme and Microbial Technology* 39:474-480.
- Kimmel GA, NG Petrik, Z Dohnalek, and BD Kay. 2006. "Layer-by-Layer Growth of Thin Amorphous Solid Water Films on Pt(111) and Pd(111)." *Journal of Chemical Physics* 125(4):044713.
- Kittle-Godfrey A and M Cafiero. 2006. "Properties, Dynamics, and Electronic Structure of Atoms and Molecules Evaluation of DFT Methods for Computing the Interaction Energies of Homomolecular and Heteromolecular Dimers of Monosubstituted Benzene." *International Journal of Quantum Chemistry* 106(9): 2035-2043.

- Kirkpatrick R, T Masiello, A Weber, and JW Nibler. 2006. "Coherent Raman Spectra of the nu(1) Mode of (BF₃)-B-10 and (BF₃)-B-11." *Journal of Molecular Spectroscopy* 237(1):97-103.
- Kollas AC, D Domin, G Hill, M Frenklach, and WA Lester Jr. 2006. "Quantum Monte Carlo Study of Small Hydrocarbon Atomization Energies." *Molecular Physics* 104(3):467-475.
- Krstic P, RJ Harrison, and BG Sumpter. 2006. "Excited State Quantum-Classical Molecular Dynamics." *Physica Scripta* T124:101-107.
- Krupka KM, HT Schaef, BW Arey, SM Heald, WJ Deutsch, MJ Lindberg, and KJ Cantrell. 2006. "Residual Waste from Hanford Tanks 241-C-203 and 241-C-204: I. Solids Characterization." *Environmental Science and Technology* 40(12):3749-3754.
- Kugai J, V Subramani, C Song, MH Engelhard, and Y Chin. 2006. "Effects of Nanocrystalline CeO₂ Supports on the Properties and Performance of Ni-Rh Bimetallic Catalyst for Oxidative Steam Reforming of Ethanol." *Journal of Catalysis* 238(2):430-440.
- Kukkadapu RK, JM Zachara, JK Fredrickson, JP McKinley, DW Kennedy, SC Smith, and H Dong. 2006. "Reductive Biotransformation of Fe in Shale-Limestone Saprolite Containing Fe(III) Oxides and Fe(II)/Fe(III) Phyllosilicates." *Geochimica et Cosmochimica Acta* 70(14):3662-3676.
- Kwak JH, JE Herrera, JZ Hu, Y Wang, and CHF Peden. 2006. "A New Class of Highly Dispersed VO_x Catalysts on Mesoporous Silica: Synthesis, Characterization, and Catalytic Activity in the Partial Oxidation of Ethanol." *Applied Catalysis, A, General* 300(2):109-119
- Larsen FH, I Farnan, and AS Lipton. 2006. "Separation of ⁴⁷Ti and ⁴⁹Ti Solid-State NMR Lineshapes by Static QCPMG Experiments at Multiple Fields." *Journal of Magnetic Resonance* 178(2):228-236.
- Laskin A, JP Cowin, and MJ Iedema. 2006. "Analysis of Individual Environmental Particles Using Modern Methods of Electron Microscopy and X-Ray Microanalysis." *Journal of Electron Spectroscopy and Related Phenomena* 150(2-3):260-274.
- Laskin A, H Wang, WH Robertson, JP Cowin, MJ Ezell, and BJ Finlayson-Pitts. 2006. "A New Approach to Determining Gas-Particle Reaction Probabilities and Application to the Heterogeneous Reaction of Deliquesced Sodium Chloride Particles with Gas-Phase Hydroxyl Radicals." *Journal of Physical Chemistry A* 110(36):10619-10627.
- Laskin J. 2006. "Energetics and Dynamics of Fragmentation of Protonated Leucine Enkephalin from Time- and Energy-Resolved Surface-Induced Dissociation Studies." *Journal of Physical Chemistry A* 110(27):8554-8562.
- Laskin J, TH Bailey, and JH Futrell. 2006. "Mechanisms of Peptide Fragmentation from Time- and Energy-Resolved Surface-Induced Dissociation Studies: Dissociation of Angiotensin Analogs." *International Journal of Mass Spectrometry* 249:462-472.

- Li X, B Kiran, LF Cui, and LS Wang. 2005. "Magnetic Properties in Transition-Metal-Doped Gold Clusters: M@Au₆ (M=Ti,V,Cr)." *Physical Review Letters* 95(25):253401 (pages 1-4).
- Li XS, GE Fryxell, C Wang, and J Young. 2006. "Nitrocellulose Tempered Hierarchical Pore Structure in Mesoporous Thin Films." *Inorganic Chemistry Communications* 9(1):7-9.
- Lin Y, G Liu, and J Wang. 2006. "Biosensors Fabricated through Electrostatic Assembly of Enzymes/Polyelectrolyte Hybrid Layers on Carbon Nanotubes." In *Proceedings of Nanotech 2006*, Vol. 2, M Laudon and B Romanowicz, eds., pp. 252-255, NTSI-Nanotech, Boston, Massachusetts.
- Lin YC, D Sundholm, J Juselius, LF Cui, X Li, HJ Zhai, and LS Wang. 2006. "Experimental and Computational Studies of Alkali-Metal Coinage-Metal Clusters." *Journal of Physical Chemistry A* 110(12):4244-4250.
- Liu G, and Y Lin. 2006. "Amperometric Glucose Biosensor Based on Self-Assembling Glucose Oxidase on Carbon Nanotubes." *Electrochemistry Communications* 8(2):251-256.
- Liu G, and Y Lin. 2006. "Biosensor Based on Self-Assembling Acetylcholinesterase on Carbon Nanotubes for Flow Injection/Amperometric Detection of Organophosphate Pesticides and Nerve Agents." *Analytical Chemistry* 78(3):835-843.
- Liu G, and Y Lin. 2006. "Carbon Nanotube Tempered Assembly of Protein." *Journal of Nanoscience and Nanotechnology* 6(4):948-953.
- Liu G, J Wang, S Lea, and Y Lin. 2006. "Bioassay Labels Based on Apoferritin Nanovehicles." *Chembiochem* 7(9):1315-1319.
- Liu RC, DH Hu, X Tan, and HP Lu. 2006. "Revealing Two-State Protein-Protein Interactions of Calmodulin by Single-Molecule Spectroscopy." *Journal of the American Chemical Society* 128(31):10034-10042.
- Liu T, WJ Qian, MA Gritsenko, DG Camp II, ME Monroe, RJ Moore, and RD Smith. 2005. "Human Plasma N-Glycoproteome Analysis by Immunoaffinity Subtraction, Hydrazide Chemistry, and Mass Spectrometry." *Journal of Proteome Research* 4(6):2070-2080.
- Liu T, W Qian, HM Mottaz, MA Gritsenko, AD Norbeck, RJ Moore, SO Purvine, DG Camp, II, and RD Smith. 2006. "Evaluation of Multi-Protein Immunoaffinity Subtraction Systems for Plasma Proteomics and Candidate Biomarker Discovery Using Mass Spectrometry." *Molecular & Cellular Proteomics*.
- Liu YF, W Chen, AG Joly, YQ Wang, C Pope, YB Zhang, JO Bovin, and P Sherwood. 2006. "Comparison of Water-Soluble CdTe Nanoparticles Synthesized in Air and in Nitrogen." *Journal of Physical Chemistry B* 110(34):16992-17000.

- Lumetta GJ, BK McNamara, TL Hubler, DW Wester, J Li, and SL Latesky. 2006. "Potential Application of Kläui Ligands in Actinide Separations." In *Separations for the Nuclear Fuel Cycle in the 21st Century*, pp. 201-218, American Chemical Society, Washington, D.C.
- Luo Q, K Tang, F Yang, A Elias, Y Shen, RJ Moore, R Zhao, KK Hixson, SS Rossie, and RD Smith. 2006. "More Sensitive and Quantitative Proteomic Measurements Using Very Low Flow Rate Porous Silica Monolithic LC Columns with Electrospray Ionization-Mass Spectrometry." *Journal of Proteome Research* 5(5):1091-1097.
- Maki A, JKG Watson, T Masiello, and TA Blake. 2006. "Observation of a Forbidden E"-A'1 Infrared Transition in $^{11}\text{BF}_3$." *Journal of Molecular Spectroscopy* 238(2):135-144.
- Marshall MJ, AS Beliaev, A Dohnalkova, DW Kennedy, L Shi, Z Wang, MI Boyanov, B Lai, KM Kemner, JS Mclean, SB Reed, DE Culley, VL Bailey, CJ Simonson, D Saffarini, MF Romine, JM Zachara, and JK Fredrickson. 2006. "c-Type Cytochrome-Dependent Formation of U(IV) Nanoparticles by *Shewanella oneidensis*." *PloS Biology* 4(8):1324-1333.
- Matulis VE and OA Ivaskovich. 2006. "Comparative DFT Study of Electronic Structure and Geometry of Copper and Silver Clusters: Interaction with NO Molecule." *Computational Materials Science* 35(3):261-271.
- Matus MH, J. Garza, and M Galvan. 2006. "Effect of Double Bonds on the Conducting Properties of Ciguatoxin 3C and Tetrahydropyrane-Based Polymers: A Theoretical Study." *Journal of Physical Chemistry B* 110(3):1172-1178.
- Migliore A, S. Corni, R Di Felice, and E Molinari. 2006. "First-Principles Density-Functional Theory Calculations of Electron-Transfer Rates in Azurin Dimers." *Journal of Chemical Physics* 124(6):064501.
- Minard KR, DR Einstein, RE Jacob, S Kabilan, AP Kuprat, C Timchalk, LL Trease, and RA Corley. 2006. "Application of Magnetic Resonance (MR) Imaging for the Development and Validation of Computational Fluid Dynamic (CFD) Models of the Rat Respiratory System." *Inhalation Toxicology* 18(10):787-794.
- Moision RM and PB Armentrout. 2006. "The Special Five-Membered Ring of Proline: An Experimental and Theoretical Investigation of Alkali Metal Cation Interactions with Proline and Its Four- and Six-Membered Ring Analogues." *Journal of Physical Chemistry A* 110:3933-3946.
- Mulas G, G Mallocci, C Joblin, and D Toublanc. 2006. "Estimated IR and Phosphorescence Emission Fluxes for Specific Polycyclic Aromatic Hydrocarbons in the Red Rectangle." *Astronomy & Astrophysics* 446(2):537-549.
- Nie J, HY Xiao, X Zu, and F Gao. 2006. "First-Principles Study of Sb Adsorption on Ag (110)(2×2)." *Chemical Physics* 326(2-3):583-588.

- Nie L, G Wu, FJ Brockman, and W Zhang. 2006. "Integrated Analysis of Transcriptomic and Proteomic Data of *Desulfovibrio vulgaris*: Zero-Inflated Poisson Regression Models to Integrate and Interpret Microarray and Proteomic Data." *Bioinformatics* 22(13):1641-1647.
- Nielsen I and MD Allendorf. 2006. "Thermochemistry of the Chromium Hydroxides Cr(OH)_n, n = 2-6, and the Oxyhydroxide CrO(OH): *Ab Initio* Predictions." *Journal of Physical Chemistry A* 110:4093-4099.
- Nieplocha J, BJ Palmer, V Tipparaju, M Krishnan, HE Trease, and E Apra. 2006. "Advances, Applications, and Performance of the Global Arrays Shared Memory Programming Toolkit." *International Journal of High Performance Computing Applications* 20(2):230-231.
- Oehmen CS and J Nieplocha. 2006. "ScalabLAST: A Scalable Implementation of BLAST for High-Performance, Data-Intensive Bioinformatics Analysis." *IEEE Transactions on Parallel and Distributed Systems* 17(8):740-749.
- Oehmen CS, T Straatsma, GA Anderson, G Orr, BM Webb-Robertson, RC Taylor, RW Mooney, DJ Baxter, DR Jones, and DA Dixon. 2006. "New Challenges Facing Integrative Biological Science in the Post-Genomic Era." *Journal of Biological Systems* 14(2):275-293.
- Oostrom M, JH Dane, and TW Wietsma. 2006. "A Review of Multidimensional, Multifluid Intermediate-Scale Experiments: Nonaqueous Phase Liquid Dissolution and Enhanced Remediation." *Vadose Zone Journal* 5:570-598.
- Page JS, AV Tolmachev, K Tang, and RD Smith. 2006. "Theoretical and Experimental Evaluation of the Low M/Z Transmission of an Electrodynamic Ion Funnel." *Journal of the American Society for Mass Spectrometry* 17(4):586-592.
- Pan DH, N Klymyshyn, DH Hu, and HP Lu. 2006. "Tip-Enhanced Near-Field Raman Spectroscopy Probing Single Dye-Sensitized TiO₂ Nanoparticles." *Applied Physics Letters* 88(9):093121.
- Patwardhan AJ, EF Strittmatter, DG Camp II, RD Smith, and M Pallavicini. 2005. "Comparison of Normal and Breast Cancer Cell Lines using Proteome, Genome, and Interactome Data." *Journal of Proteome Research* 4(6):1952-1960.
- Patwardhan AJ, EF Strittmatter, DG Camp, II, RD Smith, and M Pallavicini. 2006. "Quantitative Proteome Analysis of Breast Cancer Cell Lines using ¹⁸O-Labeling and the Accurate Mass and Time Tag Strategy." *Proteomics* 6(9):2903-2915.
- Petrik NG, AG Kavetsky, and GA Kimmel. 2006. "Electron-Stimulated Production of Molecular Oxygen in Amorphous Solid Water." *Journal of Physical Chemistry B* 110(6):2723-2731.

Petritis K, LJ Kangas, B Yan, EF Strittmatter, ME Monroe, W Qian, JN Adkins, RJ Moore, Y Xu, MS Lipton, DG Camp, II, and RD Smith. 2006. "Improved Peptide Elution Time Prediction for Reversed-Phase Liquid Chromatography-MS by Incorporating Peptide Sequence Information." *Analytical Chemistry* 78(14):5026-5039.

Piecuch P, S Hirata, K Kowalski, PD Fan, and TL Windus. 2006. "Automated Derivation and Parallel Computer Implementation of Renormalized and Active-Space Coupled-Cluster Methods." *International Journal of Quantum Chemistry* 106(1):79-97.

Pophristic V, S Vemparala, I Ivanov, Z Liu, ML Klein, and WF DeGrado. 2006. "Controlling the Shape and Flexibility of Arylamides: A Combined *Ab Initio*, *Ab Initio* Molecular Dynamics, and Classical Molecular Dynamics Study." *Journal of Physical Chemistry B* 110:3517-3526.

Punnoose A, MH Engelhard, and JS Hays. 2006. "Dopant Distribution, Oxygen Stoichiometry and Magnetism of Nanoscale Sn_{0.99}Co_{0.01}." *Solid State Communications* 139(8):434-438.

Ramirez-Solis A, R Poteau, and JE Daudey. 2006. "The Electronic Spectrum of AgCl₂: *Ab initio* Benchmark Versus Density-Functional Theory Calculations on the Lowest Ligand-Field States Including Spin-Orbit Effects." *Journal of Chemical Physics* 124(3):034307 (pages 1 – 10).

Raugei S and P Carloni. 2005. "Structure and Function of Vanadium Haloperoxidases." *Journal of Physical Chemistry B* 110(8):3747-3758.

Redington RL, TE Redington, and RL Sams. 2006. "Quantum Tunneling in the Midrange Vibrational Fundamentals of Tropolone." *Journal of Physical Chemistry A* 110(31):9633-9642.

Roberts AG, MD Diaz, JN Lampe, LM Shireman, JS Grinstead, MJ Dabrowski, JT Pearson, MK Bowman, WM Atkins, and AP Campbell. 2006. "NMR Studies of Ligand Binding to P450eryF Provides Insight into the Mechanism of Cooperativity." *Biochemistry* 45(6):1673-1684.

Roh H, Y Wang, DL King, A Platon, and Y Chin. 2006. "Low Temperature and H₂ Selective Catalysts for Ethanol Steam Reforming." *Catalysis Letters* 108(1-2):15-19.

Roh Y, H Gao, H Vali, DW Kennedy, Z Yang, W Gao, A Dohnalkova, RD Stapleton, J Moon, TJ Phelps, JK Fredrickson, and J Zhou. 2006. "Metal Reduction and Iron Biomineralization by a Psychrotolerant Fe(III)-Reducing Bacterium, *Shewanella* sp. Strain PV-4." *Applied and Environmental Microbiology* 72(5):3236-3244.

Rudra I, Q Wu, and T Van Voorhis. 2006. "Accurate Magnetic Exchange Couplings in Transition-Metal Complexes from Constrained Density-Functional Theory." *Journal of Chemical Physics* 124(2):024103.

Sacksteder CA, W Qian, TV Knyushko, HH Wang, MH Chin, DG Camp, II, RD Smith, D Smith, TC Squier, and DJ Bigelow. 2006. "Endogenously Nitrated Proteins in Mouse Brain: Links to Neurodegenerative Disease." *Biochemistry* 45(26):8009-8022.

Sacksteder CA, JE Whittier, Y Xiong, J Li, NA Galeva, ME Jacoby, SO Purvine, TD Williams, MC Rechsteiner, DJ Bigelow, and TC Squier. 2006. "Tertiary Structural Rearrangements upon Oxidation of Methionine145 in Calmodulin Promotes Targeted Proteasomal Degradation." *Biophysical Journal* 91(4):1480-1493.

Salcedo D, TB Onasch, K Dzepina, MR Canagaratna, Q Zhang, JA Huffman, PF DeCarlo, JT Jayne, P Mortimer, DR Worsnop, CE Kolb, KS Johnson, B Zuberi, LC Marr, R Volkamer, LT Molina, MJ Molina, B Cardenas, RM Bernabe, C Marquez, JS Gaffney, NA Marley, A Laskin, V Shutthanandan, Y Xie, W Brune, R Lesher, T Shirley, and JL Jimenez. 2006. "Characterization of Ambient Aerosols in Mexico City during the MCMA-2003 Campaign with Aerosol Mass Spectrometry: Results from the CENICA Supersite." *Atmospheric Chemistry and Physics* 6:925-946.

Sanchez R, W Nortershauser, G Ewald, D Albers, J Behr, P Bricault, BA Bushaw, A Dax, J Dilling, M Dombsky, GWF Drake, S Gotte, R Kirchner, HJ Kluge, T Kuhl, J Lassen, CDP Levy, MR Pearson, EJ Prime, V Ryjkov, A Wojtaszek, ZC Yan, and C Zimmermann. 2006. "Nuclear Charge Radii of $^{9,11}\text{Li}$: The Influence of Halo Neutrons." *Physical Review Letters* 96(3):033002 (pages 1-4).

Sanchez-Mori P, AJ Cohen, and W Yang. 2006. "Self-Interaction-Free Exchange-Correlation Functional for Thermochemistry and Kinetics." *Journal of Chemical Physics* 124(9):91102.

Sanville E, A Burnin, and JJ BelBruno. 2006. "Experimental and Computational Study of Small ($n = 1\text{-}16$) Stoichiometric Zinc and Cadmium Chalcogenide Clusters." *Journal of Physical Chemistry A* 110(7):2378-2386.

Saraf LV, DE McCready, V Shutthanandan, CM Wang, MH Engelhard, and S Thevuthasan. 2006. "Correlation Among Channeling, Morphological, and Micro-structural Properties in Epitaxial CeO_2 Films." *Electrochemical and Solid-State Letters* 9(5):J17-J20.

Schmitt S, H Prokisch, T Schlunck, DG Camp II, U Ahting, T Waizenegger, C Scharfe, T Meitinger, A Imhof, W Neupert, PJ Oefner, and D Rapaport. 2006. "Proteome Analysis of Mitochondrial Outer Membrane from *Neurospora crassa*." *Proteomics* 6(1):72-80.

Schryver JC, CC Brandt, SM Pfiffner, T Palumbo, AD Peacock, DC White, JP McKinley, and PE Long. 2006. "Application of Nonlinear Analysis Methods for Identifying Relationships between Microbial Community Structure and Groundwater Geochemistry." *Microbial Ecology* 51(2006):177-188.

Schumann PG, KDA Wendt, and BA Bushaw. 2005. "High-Resolution Triple-Resonance Autoionization of Uranium Isotopes." *Spectrochimica Acta Part B: Atomic Spectroscopy* 60(11):1402-1411.

Seabaugh JL, H Dong, RK Kukkadapu, DD Eberl, JP Morton, and J Kim. 2006. "Microbial Reduction of Fe(III) in the Fithian and Muloorina Illites: Contrasting Extents and Rates of Bioreduction." *Clays and Clay Minerals* 54(1):67-79.

Shen Y, J Kim, EF Strittmatter, JM Jacobs, DG Camp II, R Fang, N Tolic, RJ Moore, and RD Smith. 2005. "Characterization of the Human Blood Plasma Proteome." *Proteomics* 5(15):4034-4045.

Shi L, B Chen, Z Wang, DA Elias, MU Mayer, YA Gorby, S Ni, BH Lower, DW Kennedy, DS Wunschel, HM Mottaz, MJ Marshall, EA Hill, AS Beliaev, JM Zachara, JK Fredrickson, and TC Squier. 2006. "Isolation of High-Affinity Functional Protein Complex between OmcA and MtrC: Two Outer Membrane Decaheme c-type Cytochromes of *Shewanella oneidensis* MR-1." *Journal of Bacteriology* 188(13):4705-4714.

Shi L, JN Adkins, JR Coleman, AA Schepmoes, A Dohnalkova, HM Mottaz, AD Norbeck, SO Purvine, NP Manes, HS Smallwood, HH Wang, J Forbes, P Gros, S Uzzau, KD Rodland, F Heffron, RD Smith, and TC Squier. 2006. "Proteomic Analysis of *Salmonella enterica Serovar Typhimurium* Isolated from RAW 264.7 Macrophages: Identification of a Novel Protein that Contributes to the Replication of *Serovar typhimurium* Inside Macrophages." *Journal of Biological Chemistry* 281:29131-29140.

Shishkin O, GV Palamarchuk, L Gorb, and J Leszczynski. 2006. "Intramolecular Hydrogen Bonds in Canonical 2'-Deoxyribonucleotides: An Atoms in Molecules Study." *Journal of Physical Chemistry B* 110:4413-4422.

Shumate WJ, DL Mattern, A Jaiswal, DA Dixon, T White, J Burgess, A Honciuc, and RM Metzger. 2006. "Spectroscopy and Rectification of Three Donor-Sigma-Acceptor Compounds, Consisting of a One-Electron Donor (Perylene or Ferrocene), a One-Electron Acceptor (Perylenebisimide), and a C-19 Swallowtail." *Journal of Physical Chemistry* 110(23):11146-11159.

Shvartsburg AA, SV Mashkevich, and RD Smith. 2006. "Feasibility of Higher-Order Differential Ion Mobility Separations Using New Asymmetric Waveforms." *Journal of Physical Chemistry A* 110(8):2663-2673.

Simner SP, MD Anderson, MH Engelhard, and JW Stevenson. 2006. "Degradation Mechanisms of La-Sr-Co-Fe-O₃ SOFC Cathodes." *Electrochemical and Solid-State Letters* 9(10):A478-A481.

Simson DC, S Ahn, L Pasa-Tolic, B Bogdanov, HM Mottaz, AN Vilkov, GA Anderson, MS Lipton, and RD Smith. 2006. "Using Size Exclusion Chromatography-RPLC and RPLC-CIEF as Two-Dimensional Separation Strategies for Protein Profiling." *Electrophoresis* 27(13):2722-2733. 03

Smith DM, KM Rosso, M Dupuis, M Valiev, and T Straatsma. 2006. "Electronic Coupling between Heme Electron-Transfer Centers and Its Decay with Distance Depends Strongly on Relative Orientation." *Journal of Physical Chemistry B* 110(31):15582-15588.

Smith RS, T Zubkov, and BD Kay. 2006. "The Effect of the Incident Collision Energy on the Phase and Crystallization Kinetics of Vapor Deposited Water Films." *Journal of Chemical Physics* 124(11):114710 (pages 1-7).

Springer DL, M Ahram, JN Adkins, LE Kathmann, and JH Miller. 2005. "Characterization of Medium Conditioned by Irradiated Cells Using Proteome-Wide, High-Throughput Mass Spectrometry." *Radiation Research* 164(5):651-654.

Straatsma T, JA McCammon, JH Miller, PE Smith, ER Vorpagel, CF Wong, and M Zacharias. 2006. *Biomolecular Simulation of Base Excision Repair and Protein Signaling*. PNNL-15687, Pacific Northwest National Laboratory, Richland, Washington.

Stewart ML, AL Ward, and DR Rector. 2006. "A Study of Pore Geometry Effects on Anisotropy in Hydraulic Permeability Using the Lattice-Boltzmann Method." *Advances in Water Resources* 29(9):1328-1340.

Sturdy YK, C Skylaris, and DC Clary. 2005. "Torsional Anharmonicity in the Conformational Analysis of β -D-Galactose." *Journal of Physical Chemistry B* 110:3485-3492.

Su F, Y Liu, W Chen, WJ Wang, K Ding, G Li, AG Joly, and DE McCready. 2006. "Temperature and Pressure Dependences of the Copper-Related Green Emission in ZnO Microrods." *Journal of Applied Physics* 100(1):013107-1—013107-6.

Su F, B Ma, K Ding, G Li, S Wang, W Chen, AG Joly, and DE McCready. 2006. "Luminescence Temperature and Pressure Studies of Zn_2SiO_4 Phosphors Doped with Mn^{2+} and Eu^{3+} Ions." *Journal of Luminescence* 116(1-2):117-126.

Szanyi J, JH Kwak, S Burton, JA Rodriguez, and CHF Peden. 2006. "Characterization of NO_x Species in Dehydrated and Hydrated Na- and Ba-Y,FAU Zeolites Formed in NO_2 Adsorption." *Journal of Electron Spectroscopy and Related Phenomena* 150(2-3):164-170.

Tanimura K, E Inami, J Kanasaki, and WP Hess. 2006. "Two-Hole Localization Mechanism for Electronic Bond Rupture of Surface Atoms by Laser-Induced Valence Excitation of Semiconductors." *Physical Review B. Condensed Matter and Materials Physics* 74(3): Art. No. 035337.

Thompson CJ, RG Riley, JE Amonette, and PL Gassman. 2006. "Quantification of Volatile Organics in Soil Aging Experiments using Fourier Transform Infrared Spectroscopy." *Applied Spectroscopy* 60(8):914-919.

Tonkyn RG, RS Disselkamp, and CHF Peden. 2006. "Nitrogen Release from a NO_x Storage and Reduction Catalyst." *Catalysis Today* 114(1):94-101.

Van Ginhoven RM, A Chartier, C Meis, WJ Weber, and LR Corrales. 2006. "Theoretical Study of Helium Insertion and Diffusion in 3C-SiC." *Journal of Nuclear Materials* 348(1-2):51-59.

van Mourik T, PG Karamertzanis, and SL Price. 2006. "Molecular Conformations and Relative Stabilities Can Be as Demanding of the Electronic Structure Method as Intermolecular Calculations." *Journal of Physical Chemistry A* 110(1):8-12.

Vayner G, Y Alexeev, J Wang, TL Windus, and WL Hase. 2006. "Ab Initio and Analytic Intermolecular Potentials for Ar-CF₄." *Journal of Physical Chemistry A* 110(9):3174-3178.

Vazquez-Mayagoitia A, R Vargas, JA Nichols, P Fuentealba, and J Garza. 2006. "Relationship Between Singlet-Triplet Excitation Energies and the Kohn-Sham Orbitals Obtained with Potentials that Exhibit a Wrong Asymptotic Behavior." *Chemical Physics Letters* 419(1-3):207-212.

Vemparala S, I Ivanov, V Popristic, and K Spiegel. 2006. "Ab Initio Calculations of Intramolecular Parameters for a Class of Arylamide Polymers." *Journal of Computational Chemistry* 27(6):693-700.

Wander MC, SN Kerisit, KM Rosso, and MA Schoonen. 2006. "Kinetics of Triscarbonato Uranyl Reduction by Aqueous Ferrous Iron: A Theoretical Study." *Journal of Physical Chemistry A* 110(31):9691-9701.

Wang CM, J Kwak, D Kim, J Szanyi, R Sharma, S Thevuthasan, and CH Peden. 2006. "Morphological Evolution of Ba(NO₃)₂ Supported on an In Situ TEM Study." *Journal of Physical Chemistry B* 110(24):11878-11883.

Wang CM, V Shuththanadan, Y Zhang, S Thevuthasan, LE Thomas, WJ Weber, and G Duscher. 2006. "Atomic Level Imaging of Au Nanocluster Dispersed in TiO₂ and SrTiO₃." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 242(1-2):380-382.

Wang H, WJ Qian, MH Chin, VA Petyuk, RC Barry, T Liu, MA Gritsenko, HM Mottaz, RJ Moore, DG Camp II, AH Khan, DJ Smith, and RD Smith. 2006. "Characterization of the Mouse Brain Proteome Using Global Proteomic Analysis Complemented with Cysteinyl-Peptide Enrichment." *Journal of Proteome Research* 5(2):361-369.

Wang J, G Liu, and Y Lin. 2006. "Amperometric Choline Biosensor Fabricated through Electrostatic Assembly of Bienzyme/Polyelectrolyte Hybrid Layers on Carbon Nanotubes." *Analyst* 131(4):477-483.

Wang J, G Liu, and Y Lin. 2006. "Electroactive Silica Nanoparticles for Biological Labeling." *Small* 2(10):1134-1138.

Wang J, Q Lu, and HP Lu. 2006. "Single-Molecule Dynamics Reveals Cooperative Binding-Folding in Protein Recognition." *PLoS Computational Biology* 2(7):842-852.

Wang S, and HF Schaefer III. 2006. "The Small Planarization Barriers for the Amino Group in the Nucleic Acid Bases." *Journal of Chemical Physics* 124(4):044303.

Wang X, L Andrews, and J Li. 2006. "Experimental and Theoretical Investigations of Infrared Spectra and Electronic Structures of the U(OH)₂, UO₂(OH), and UO₂(OH)₂ Molecules." *Inorganic Chemistry* 45(10):4157-4166.

Wang XB, HK Woo, X Huang, MM Kappes, and LS Wang. 2006. "Direct Experimental Probe of the On-Site Coulomb Repulsion in the Doubly Charged Fullerene Anion C-70 (2-)." *Physical Review Letters* 96(14):143002

Wang XB, HK Woo, LS Wang, B Minofar, and P Jungwirth. 2006. "Determination of the Electron Affinity of the Acetyl Radical (CH₃COO) by Low-Temperature Anion Photoelectron Spectroscopy and *Ab Initio* Calculations." *Journal of Physical Chemistry A* 110(15):5047-5050.

Wang Z, AR Felmy, Y Xia, and EC Buck. 2006. "Observation of Aqueous Cm(III)/Eu(III) and UO₂²⁺ Nanoparticulates at Concentrations Approaching Solubility Limit by Laser-Induced Fluorescence Spectroscopy." *Journal of Alloys and Compounds* 418(1-2):166-170.

Waters T, XB Wang, S Li, B Kiran, DA Dixon, and LS Wang. 2005. "Electronic Structure of the Hydroxo and Methoxy Oxometalate Anions MO₃(OH)⁻ and MO₃(OCH₃)⁻ (M = Cr, Mo, and W)." *Journal of Physical Chemistry A* 109(51):11771-11780.

Waters T, XB Wang, HK Woo, and LS Wang. 2006. "Photoelectron Spectroscopy of the Bis(dithiolene) Anions [M(mnt)(2)](n-)(M = Fe-Zn; n=1, 2): Changes in Electronic Structure with Variation of Metal Center and with Oxidation." *Inorganic Chemistry* 45(15):5841-5851.

Waters T, HK Woo, XB Wang, and LS Wang. 2006. "Probing the Intrinsic Electronic Structure of the Bis(dithiolene) Anions [M(mnt)(2)](2-) and [M(mnt)(2)](1-) (M = Ni, Pd, Pt; mnt=1,2-S₂C₂(CN)(2)) in the Gas Phase by Photoelectron Spectroscopy." *Journal of the American Chemical Society* 128(13):4282-4291.

Weber KA, MM Urrutia, PF Churchill, RK Kukkadapu, and EE Roden. 2006. "Anaerobic Redox Cycling of Iron by Freshwater Sediment Microorganisms." *Environmental Microbiology* 8(1):100-113.

Whitlow HJ, Y Zhang, CM Wang, DE McCready, T Zhang, and Y Wu. 2006. "Formation of Cobalt Silicide from Filter Metal Vacuum Arc Deposited Films." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 247(2):271-278.

Wierzchowski SJ, ZH Fang, DA Kofke, and JL Tilson. 2006. "Three-Body Effects in Hydrogen Fluoride: Survey of Potential Energy Surfaces." *Molecular Physics* 104(4):503-513.

Wind RA, JZ Hu, and PD Majors. 2006. "Localized *in vivo* Isotropic-Anisotropic Correlation ¹H NMR Spectroscopy Using Ultraslow Magic Angle Spinning." *Magnetic Resonance in Medicine* 55(1):41-49.

- Woo HK, WB Wang, KC Lau, and LS Wang. 2006. "Low-Temperature Photoelectron Spectroscopy of Aliphatic Dicarboxylate Monoanions, HO₂C(CH₂)_nCO₂⁻ (*n* = 1-10): Hydrogen Bond Induced Cyclization and Strain Energies." *Journal of Physical Chemistry A* 110(25):7801-7805.
- Woo HK, XB Wang, B Kiran, and LS Wang. 2005. "Temperature-Dependent Photoelectron Spectroscopy of Methyl Benzoate Anions: Observation of Steric Effect in O-Methyl Benzoate." *Journal of Physical Chemistry A* 109(50):11395-11400.
- Wu Q, and T Van Voorhis. 2006. "Direct Calculation of Electron Transfer Parameters through Constrained Density Functional Theory." *Journal of Physical Chemistry A* 110(29):9212-9218.
- Xantheas SS, and TA Blake. 2006. "Structure, Vibrational Spectra and Ring Puckering Barrier of Cyclobutane." *Journal of Physical Chemistry A* 110:10487-10494.
- Xia Y, NJ Hess, and AR Felmy. 2006. "Stability Constants of Technetium (IV) Oxalate Complexes as a Function of Ionic Strength." *Radiochimica Acta* 94(3):137-141.
- Xiao HY, XT Zu, YF Zhang, and F Gao. 2006. "Adsorption of Alkali Metals on Ge(001)(2×1) Surface." *Chemical Physics Letters* 417(1-3):6-10.
- Xiao HY, X Zu, Y Zhang, and F Gao. 2006. "Atomic and Electronic Structures of Rubidium Adsorption on Si(001)(2 x 1) Surface: Comparison with Cs/Si(001) Surface." *Chemical Physics* 323(2-3):383–390.
- Xiong G, AG Joly, KM Beck, WP Hess, MD Cai, SC Langford, and JT Dickinson. 2006. "In Situ Photoelectron Emission Microscopy of a Thermally Induced Martensitic Transformation in a CuZnAl Shape Memory Alloy." *Applied Physics Letters* 88(9):091910 (pages 1-3).
- Xiong G, AG Joly, GR Holtom, CM Wang, DE McCready, KM Beck, and WP Hess. 2006. "Excited Carrier Dynamics of α -Cr₂O₃/ α -Fe₂O₃ Core-Shell Nanostructures." *Journal of Physical Chemistry B* 110(34):16937-16940. 7
- Yadav NN, S Maheswaran, V Shuthanandan, S Thevuthasan, TR Hart, H Ngo, and S Vigneswaran. 2006. "Comparison of Analytical Techniques for Analysis of Arsenic Adsorbed on Carbon." *Water Quality Research Journal of Canada* 41(2):185-189.
- Yan P, Y Xiong, B Chen, S Negash, TC Squier, and MU Mayer. 2006. "Fluorophore-Assisted Light Inactivation of Calmodulin Involves Singlet-Oxygen Mediated Cross-Linking and Methionine Oxidation." *Biochemistry* 45(15):4736-4748.
- Yang F, DL Stenoien, EF Strittmatter, J Wang, L Ding, MS Lipton, ME Monroe, CD Nicora, MA Gritsenko, K Tang, R Fang, JN Adkins, DG Camp, II, DJ Chen, and RD Smith. 2006. "Phosphoproteome Profiling of Human Skin Fibroblast Cells in Response to Low- and High-Dose Irradiation." *Journal of Proteome Research* 5(5):1252-1260.

- Zhai HJ, LS Wang, DY Zubarev, and AI Boldyrev. 2006. "Gold Apes Hydrogen. The Structure and Bonding in the Planar B₇Au₂- and B₇Au₂ Clusters." *Journal of Physical Chemistry A* 110(5):1689-1693.
- Zhang L, M DeRider, MA McCornack, C Jao, N Isern, T Ness, R Moyer, and PJ LiWang. 2006. "Solution Structure of the Complex Between Poxvirus-Encoded CC Chemokine Inhibitor vCCI and Human MIP-1 β " *Proceedings of the National Academy of Sciences of the United States of America* 103(38): 13985-13990.
- Zhang W, MA Gritsenko, RJ Moore, DE Culley, L Nie, K Petritis, EF Strittmatter, DG Camp, II, RD Smith, and FJ Brockman. 2006. "A Proteomic view of Desulfovibrio vulgaris Metabolism as Determined by Liquid Chromatography Coupled with Tandem Mass Spectrometry." *Proteomics* 6(15):4286-4299
- Zhang Y, WJ Weber, V Shutthanandan, and S Thevuthasan. 2006. "Non-linear Damage Accumulation in Au-Irradiated SrTiO₃." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 251(1):127-132.
doi:10.1016/j.nimb.2006.05.018
- Zhang Y, WJ Weber, DA Grove, J Jensen, and G Possnert. 2006. "Electronic Stopping Powers for Heavy Ions in Niobium and Tantalum Pentoxides." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 250(1-2):62-65.
doi:10.1016/j.nimb.2006.04.148
- Zhang Y, J Jensen, G Possnert, DA Grove, DE McCready, BW Arey, and WJ Weber. 2006. "Electronic Stopping Forces of Heavy Ions in Metal Oxides." *Nuclear Instruments and Methods in Physics Research. Section B, Beam Interactions with Materials and Atoms* 249(1-2):18-21.
doi:10.1016/j.nimb.2006.03.013
- Zhang ZR, O Bondarchuk, JM White, BD Kay, and Z Dohnalek. 2006. "Imaging Adsorbate O-H Bond Cleavage: Methanol on TiO₂(110)." *Journal of the American Chemical Society* 128(13):4198-4199.
- Zhao HB, RG Tonkyn, SE Barlow, BE Koel, and CHF Peden. 2006. "Catalytic Oxidation of HCN over a 0.5% Pt/Al₂O₃ Catalyst." *Applied Catalysis B-Environmental* 65(3-4):282-290.
- Zhao H, RG Tonkyn, SE Barlow, CHF Peden, and BE Koel. 2006. "Fractional Factorial Study of HCN Removal over a 0.5% Pt/Al₂O₃ Catalyst: Effects of Temperature, Gas Flow Rate, and Reactant Partial Pressure." *Industrial & Engineering Chemistry Research* 45(3):934-939.
- Zheng F, DL Baldwin, LS Fifield, NC Anheier, Jr., CL Aardahl, and JW Grate. 2006. "Single-Walled Carbon Nanotube Paper as a Sorbent for Organic Vapor Preconcentration." *Analytical Chemistry* 78(7):2442-2446.
- Zubarev DY, AN Alexandrova, AI Boldyrev, LF Cui, X Li, and LS Wang. 2006. "On the Structure and Chemical Bonding of Si₆²⁻ and Si₆²⁻ in NaSi₆⁻ upon Na⁺ Coordination." *Journal of Chemical Physics* 124(12):124305 (pages 1-13).

Zubarev DY, AI Boldyrev, X Li, LF Cui, and LS Wang. 2005. "Chemical Bonding in Si₅²⁻ and NaSi₅⁻ via Photoelectron Spectroscopy and *ab initio* Calculations." *Journal of Physical Chemistry A* 109(50):11385-11394.

Zubarev DY, AI Boldyrev, X Li, and LS Wang. 2006. "Observation of Triatomic Species with Conflicting Aromaticity: AlSi²⁻ and AlGe²⁻." *Journal of Physical Chemistry B* 110(20):9743-9746.

Zubarev DY, J Li, LS Wang, and AI Boldyrev. 2006. "Theoretical Probing of Deltahedral Closo-AuroBoranes B_xAu_x2 (x = 5-12)." *Inorganic Chemistry* 45(14):5269-5271.