Curriculum Vitae

Aurora Evelyn Clark

DOB: 12/12/1976 Fresno, CA

Address:
Washington State University
Department of Chemistry
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Education

Ph.D. Physical Chemistry, Indiana University, *Summa cum Laude*, April 2003
(Prof.'s Ernest R. Davidson and Jeffrey M. Zaleski, advisors)

B.S. Chemistry, Central Washington University,
Douglas Honors College, *Summa cum Laude* June 1999

Professional Experience

07/2014 – present	Director, Materials Science and Engineering Program Washington State University
08/2011-present	Associate Professor Chemistry Department Washington State University
08/2005-08/2011	Assistant Professor Chemistry Department Washington State University
07/2003-06/2005	Directors Postdoctoral Fellow, Los Alamos National Laboratory Theoretical Division, Physics and Chemistry of Materials (Dr.'s Rich Martin and Jeff Hay, advisors)

Research Interests

Our area of expertise lies in the synergistic use of Density Functional Theory and Molecular Dynamics to understand the physical properties of and reactions within complex solution phase environments. We are particularly interested in applications related to interfacial chemistry, such as in catalysis, environmental remediation, and separations. As a natural extension of these applications we also develop new software and in recent years have pioneered the development of Intermolecular Network Theory as a mechanism for understanding the collective structure and dynamics of solvents, the solvation environment about a solute and its role in reactivity.

Honors and Awards

2015 WSU College of Arts and Sciences Mid-Career Award

2014 Volunteer of the Year, Washington Idaho Border Section of the American Chemical Society
2009 WSU Undergraduate Research Excellence Mentor Award
2009 American Chemical Society HP Junior Faculty Award (Comp division)
2008 WSU College of Sciences Young Faculty Performance Award
2008 American Chemical Society PROGRESS/Dreyfus Lectureship Award
2007 DOE Nuclear Science, Engineering and Health Physics Junior Faculty Award

Professional Societies

1. American Chemical Society, Member
    a. Computers in Chemistry Division, Member
    b. Physical Chemistry Division, Member
    c. *2012-2013 Chair*, Washington Idaho Border Section
2. American Physical Society, Member
    a. Division of Computational Physics, Member at Large 2016-2019
3. American Nuclear Society, Member
4. Materials Research Society, Member

Publications (h-factor 24, > 1400 citations)

Research conducted by a
**High school student
*Undergraduate student
#Graduate student
+Post Doctoral researcher

Journal Impact Factor denoted by (*I. F.*)

67. Parmar, P.;+ Ghadar, Y.;# Henson, N.; Clark, A. E. Aqueous Solvation of Early Trivalent Actinide Ions: Comparisons of Thermodynamic, Structural, and Dynamic Features From Classical Potentials. *Journal of Physical Chemistry B*, **2015**, *submitted.*

66. Wu, J.;+ Kucukkal, M.;+ Clark, A. E. H_2 Adsorbed Site-to-Site Electronic Delocalization Within IRMOF-1: Understanding Non-negligible Interactions at High Pressure. *Journal of Physical Chemistry C* **2015**, *submitted (I.F. 4.835)*

65. Kelley, M.;# Donley, A.;# Clark, S.; Clark, A. E. Structure and Dynamics of NaCl Ion Pairing in Solutions of Water and Methanol *Journal of Physical Chemistry B* **2015** DOI 10.1021/acs.jpcb.5b07492 *(I. F. 3.377)*

64. Knorr, F.; McHale, J. L.; Clark, A. E.; Marchioro, A.; Moser, J. –E. Dynamics of Interfacial Electron Transfer from Betanin to Nanocrystalline TiO_2: The Pursuit of Two-Electron Injection. *Journal of Physical Chemistry C* **2015** *119*, 19030–19041 *(I. F. 4.835)*

63. Zhou, T.#; Ozkanlar, A.+; Clark, A. E. Understanding Hydrogen Bond Reorientation Dynamics in Water: Two Classes of Reorientation Processes, *Journal of Chemical Physics* **2015** *submitted (I. F. 4.2)*

62. Ghadar, Y.[#]; Christiansen, S. L.[*]; Clark, A. E. Influence of Aqueous Ionic Strength Upon Liquid:Liquid Interfacial Structure and Dynamics, *Fluid Phase Equilibria*, **2015**, *Invited article – special issue Aqueous Solutions: Bulk Fluids and Interfaces*. DOI 10.1016/j.fluid.2015.07.013 *(I.F. 2.241)*.

61. Clark, A. E.; Samuels, A.[#]; Wisuri, K.[*]; Landstrom, S.[*]; Saul, T.[**] Sensitivity of Solvation Environment to Oxidation State and Position in the Early Actinide Period, *Inorganic Chemistry*, **2015**, *54*, 6216-6225*. (I.F. 4.794*)

60. Ghadar, Y.[#]; Parmar, P.;[+] Samuels, A.;[#] Clark, A. E. Solutes at the Liquid:Liquid Phase Boundary – Solubility and Solvent Conformational Response Alter Interfacial Microsolvation Reactions, *Journal of Chemical Physics*, **2015**, *142* , 104707*. (I.F. 3.122)*

59. Samuels, A. C.[#]; Victor, E. M.[*]; Clark, A. E.; Wall. N. A. Rh(III) Extraction by Phosphinic Acids *Solvent Extraction and Ion Exchange*, **2015**, *33, 418-428*. (I.F. 2.38)

58. Parmar, P.[+]; Samuels, A.[#], Clark, A. E. Applications of Polarizable Continuum Models to Determine Accurate Solution-phase Thermochemical Values Across a Broad Range of Cation Charge – The Case of U(III-VI), *Journal of Chemical Theory and Computation*, **2015**, *11*, 55-63. *(I.F. 5.389)*

57. Ozkanlar, A.; [+] Zhou, T.;[#] Clark, A. E. Towards a Unified Descriptions of Hydrogen Bond Networks of Liquid Water: A Dynamics Based Approach *Journal of Chemical Physics* **2014** *141*, 214107*. (I.F. 3.122)*

56. Samuels, A.[#]; Boele, C. A.[#]; Bennett, K. T.[#]; Clark, S. B .; Wall, N. A.; Clark, A. E. An Integrated Computational and Experimental Protocol for Understanding Rh(III) Speciation in Hydrochloric and Nitric Acid Solutions *Inorganic Chemistry* **2014** *53*, 12315-12322*. (I.F. 4.794)*

55. Parmar, P.[+], Peterson, K. A.; Clark, A. E. Static Electric Dipole Polarizabilities of $An^{5+/6+}$ and $AnO_2^{+/2+}$ (An = U, Np, and Pu) Ions *Journal of Chemical Physics*, **2014**, *141*, 234304*. (I.F. 3.122)*

54. Wang, C.;[#] Bai, P.;[#] Siepmann, I.; Clark, A. E. Deconstructing hydrogen bond networks of solvents confined in nanoporous materials: Implications for alcohol-water separation *Journal of Physical Chemistry C* **2014**, *118,* 19723-19832. *(I.F. 4.835)*

53. Yang, X.; Clark, A. E. Preferential Solvation and Crystallization/Dissolution Mechanisms in Metal Organic Frameworks *Inorganic Chemistry* **2014**, *53*, 8930-8940. (*I.F. 4.794*)

52. Ghadar, Y.[#]; Clark, A. E. Intermolecular Network Analysis of the Liquid and Vapor Interfaces of Pentane and Water: Microsolvation Does Not Trend with Interfacial Properties, *Physical Chemistry Chemical Physics*, **2014**, *16*, 12475 – 12487.;**2015**, *17*, 16646 - 16646 (*I.F. 4.2*)

51. Ozkanlar, A.[+], Kelley, M.[#], Clark, A. E. Water Organization and Dynamics on Mineral Surfaces Interrogated by Theoretical Analysis of Intermolecular Chemical Networks, *Minerals*, **2014**, *4*, 118-129. (invited article, new journal – no impact factor)

50. Hauck, B. C.[#]; Davis, E. J.[#]; Clark, A. E.; Siems, W. F.; Harden, C. S.; McHugh, V. M.; Hill, H. H. Jr. Using Ion Mobility Measurements to Determine the Water Content of a Drift Gas in Ion Mobility Spectrometry, *International Journal of Mass Spectrometry*, **2014**, *368*, 37-44. *(I. F. 2.227)*

49. Ozkanlar, A.[+]; Clark, A. E. *ChemNetworks*: A Complex Network Analysis Tool for Chemical Systems, *Journal of Computational Chemistry*, **2014**, *35*, 495-505. *(I.F.* 3.85)

48. Parmar, P. K.[+]; Peterson, K. A.; Clark, A. E. Static Electric Dipole Polarizabilities of Tri- and Tetravalent U, Np, and Pu Ions, *Journal of Physical Chemistry A,* **2013**, *117*, 11874-11880. *(I.F. 3.122)*)

47. Ozkanlar, A.[+]; Samuels, A.[#]; Clark, A. E. A Proposed Mechanism for Controlling Hydride Formation in Transition Metal Doped Mg Using an External Magnetic Field, *Chemical Physics Letters* **2013**, *560,* 10-14. (*I. F.* 2.215)

46. Kuta, J.[+]; Wang, Z.; Wisuri, K.[*]; Wander, M. C. F.[+]; Wall, N. A.; Clark, A. E. Aqueous Surface chemistry of alpha-Uranophane. *Geochimica Cosmochimica Acta*, **2013***, 103*, 184-196. (*I. F.* 4.517)

45. Ozkanlar, A.[+]; Clark, A. E. Sensitivity of the Properties of Ruthenium "Blue Dimer" to Method, Basis Set, and Continuum Model, *Journal of Chemical Physics*, **2012**, *136*, 204104. (*I.F. 3.122*)

44. Hudelson, M.; Mooney, B. L.[#]; Clark, A. E. Determining Polyhedral Arrangements of Atoms Using PageRank, *Journal of Mathematical Chem*istry **2012**, *50*, 2342. (*I.F.* 1.27)

43. Taw, F. L.[+]; Clark, A. E.[+]; Mueller, A. H.[+]; Janicke, M. T.[+]; Cantat, T.[+]; Scott, B. L.; Hay, P. J.; Hughes, R. P.; Kiplinger, J. K. Titanium(IV) Trifluoromethyl Complexes: New Perspectives on Bonding From Organometallic Fluorocarbon Chemistry, *Organometallics*, **2012**, *31*, 1484. (*I.F* 3.88)

42. Mooney, B. L.[#]; Corrales, L. R.; Clark, A. E. Novel Analysis of Cation Solvation Using Graph Theoretic Approaches, *Journal of Physical Chemistry B*, **2012**, *116*, 4263. (*I.F* 3.603)

41. Zakharova, N. L.[#]; Quinton, J.;* Crawford, C. L.[#]; Hauck, B. C.*; Hill, H. H.; Clark, A. E. An Assessment of Computational Methods for Obtaining Gas Phase Structural Information of Moderately Flexible Biomolecules from ion Mobility Spectrometry Measurements, *Journal of the American Society of Mass Spectrometry*, **2012**, *23*, 792. (*I.F* 3.830)

40. Mooney, B. L.[#]; Corrales, L. R.; Clark, A. E. *moleculaRnetworks*: An Integrated Graph Theoretic and Data Mining Tool to Explore Solvent Organization in Molecular Simulation, *Journal of Computational Chemistry*, **2012**, *33*, 853-860. (*I.F* 4.05)

39. Ghadar, Y.[#]; Clark, A. E. Coupled-cluster, Moller-Plesset (MP2), Density Fitted Local MP2, and DFT Examination of the Energetic and Structural Features of Hydrophobic Solvation: Water and Pentane, *Journal of Chemical Physics*, **2012**, *136*, 054305. (Featured article, one of the top 20 most downloaded in February 2012) (*I.F* 3.33)

38. Ozkanlar, A.[+]; Cape, J.[+]; Hurst, J.; Clark, A. E. "Covalent Hydration" Reactions in Model Monomeric Ru 2,2'-bipyridine Catalysts: Thermodynamic Favorability as a Function of Metal Oxidation and Overall Spin States, *Inorganic Chemistry*, **2011**, *50*, 8177-8187. (*I.F* 4.326)

37. Hurst, J. K.; Clark, A. E. Mechanisms of Water Oxidation Catalyzed by Ruthenium Coordination Complexes, *Progress in Inorganic Chemistry*, **2011**, *57*, 1 - 54. (*I.F.* 9.33)

36. Kuta, J.[+]; Wander, M. C. F.[+]; Wang, Z.; Jian S.[+]; Wall, N. A.; Clark, A. E. Trends in Ln(III) Sorption to Quartz Assessed by Molecular Dynamics Simulations and Laser Induced Fluorescence Studies, *Journal of Physical Chemistry C*, **2011**, *115*, 21120-21127. (*I.F* 4.524)

35. Kuta, J.[+]; Clark, A. E. Trends in Aqueous Hydration Across the 4f Period Assessed by Reliable Computational Methods, *Inorganic Chemistry* **2010**, *49*, 7808-7817. (*I.F* 4.326)

34. Takami, T.; Clark, A. E.; Mazur, U.; Hipps, K. W. Building Self-Assembled Molecular Layers with Axially Substituted Titanium Phthalocyanines, *Langmuir*, **2010**, *26*, 12709-12715. (*I.F* 4.269)

33. Waldher, B.[*]; Kuta, J.[+]; Chen, S.[#]; Henson, N.; Clark, A. E. ForceFit: A Code to Fit Classical Force Fields to Quantum Mechanical Potential Energy Surfaces, *Journal of Computational Chemistry* **2010**, *31*, 2307-2316. (*I.F* 4.05)

32. Wander, M. C. F.[+]; Clark, A. E. Gradient Fit Functions for 2-Body Potential Energy Surfaces Based Upon a Harmonic Series, *Molecular Simulation* **2010**, *36,* 335-340. (*I.F* 1.215)

31. Kvamme, B.[*]; Wander, M. C. F.[+]; Clark, A. E. The Role of Basis Set Superposition Error in Water Addition Reactions to Ln(III). *International Journal of Quantum Chemistry* **2009** *109*, 2474 – 2481. (*I.F* 1.37)

30. Wander, M. C. F.[+]; Kubicki, J. D.; Clark, A. E.; Schoonen, M. A. Ferrous Iron Reduction of Superoxide – a Proton Coupled Electron Transfer 4-Point Test. *Journal of Physical Chemistry A* **2009** *113,* 1020-1025*.* (*I.F* 2.732)

29. Bhattacharrryya, S.; Clark, A. E.; Pink, M.; Zaleski, J. M. Structure Modulated Electronic Structure Contributions to Metalloenediyne Reactivity: Synthesis and Thermal Bergman Cyclization of MLX_2 Compounds. *Inorganic Chemistry* **2009,** *48*, 3916–3925. *(cover article)* (*I.F* 4.326)

28. Clark, A. E.; Bhattacharryya, S.; Zaleski, J. M. Electronic Effects Induced by Halogen Ligation to Metalloenediynes. *Inorganic Chemistry* **2009**, *48*, 3926–3933. (*cover article)* (*I.F* 4.326)

27. Wander, M. C. F.[+]; Clark, A. E. Structural and Dielectric Properties of Quartz-Water Interfaces. *Journal of Physical Chemistry C* **2008**, *112*, 19986-19994. (*I.F* 4.524)

26. Wander, M. C. F.[+]; Clark, A. E. Hydration Properties of Aqueous Pb(II) *Inorganic Chemistry* **2008**, *47*, 8233-8241. (*I.F* 4.326)

25. Dinescu, A.[+]; Clark, A. E. Thermodynamic and Structural Features of Aqueous Ce(III), *Journal of Physical Chemistry A* **2008***, 112*, 11198-11206*.* (*I.F* 2.732)

24. Clark, A. E. Density Functional and Basis Set Dependence of Hydrated Ln(III) Properties. *Journal of Chemical Theory and Computation* **2008**, *4,* 708-718. (*I.F* 5.138)

23. Hurst, J. K.; Cape, J. L.[+]; Clark, A. E.; Das, Samir[+]; Qin, C.[+] Mechanisms of Water Oxidation Catalyzed by Ruthenium Diimine Complexes. *Inorganic Chemistry* **2008**, *47*, 1753-1764. (*I.F* 4.326)

22. Clark, A. E.; Qin, C.[+]; Li, A. D. Q. Beyond exciton theory: A time-dependent DFT and Franck-Condon study of perylene diimide and its chromophoric dimer. *Journal of the American Chemical Soc*iety **2007**, *129*, 7586-7595. (*I.F* 9.023)

21. Peterangelo, S. C.; Hart, R. T.; Clark, A. E. Correlations between rheological properties of zinc carboxylate liquids and molecular structure. *Journal of Physical Chemistry B* **2007**, *111*, 7073-7077. (*I.F* 3.603)

20. Qin, C.[+]; Clark, A. E. DFT Characterization of the Optical and Redox Properties of Natural Pigments Relevant to Dye-Sensitized Solar Cells. *Chemical Physics Letters* **2007**, *438*, 26-30. (*I.F* 2.213)

19. Davidson, E. R.; Clark, A. E.[+] Analysis of wave functions for open-shell molecules. *Physical Chemistry Chemical Physics* **2007**, *9*, 1881-1894. (*I.F* 3.453)

18. Clark, A. E. TDDFT Studies of the Photoswitching of the Two-Photon Absorption Spectra in Stilbene, Metacyclophenadiene, and Diarylethene Chromophores. *Journal of Physical Chemistry A.* **2006**, *110*, 3790-3796. (*I.F* 2.732)

17. Bruhn, G.[*]; Davidson, E. R.; Mayer, I.; Clark, A. E. Löwdin Population Analysis With and Without Rotational Variance. *International Journal of Quantum Chemistry* **2006**, *106*, 2065-2072. (*I.F* 1.37)

16. Veauthier, J. M.[+]; Schelter, E. J.[+]; Kuehl, C. J.; Clark, A. E.; Scott, B. L.; Morris, D. E.; Martin, R. L.; Thompson, J. D.[+]; Kiplinger, J. K.; John, K. D. Ligand substituent effect observed for ytterbocene 4'-cyano-2,2':6',2' '-terpyridine, *Inorganic Chemistry* **2005**, *44*, 5911. (*I.F* 4.326)

15. Clark, A. E.[+]; Martin, R. L.; Hay, P. J.; Green, J. C.; Jantunen, K. C.; Kiplinger, J. L. Electronic structure, excited states, and photoelectron spectra of uranium, thorium, and zirconium bis(ketimido) complexes $(C_5R_5)_2M[\text{-}N{=}CPh_2]_2$ (M = Th, U, Zr; R = H, CH_3), *Journal of Physical Chemistry A*. **2005**, *109,* 5481-5491. (*I.F* 2.732)

14. Davidson, E. R.; Clark, A. E. Spin polarization and annihilation for radicals and diradicals, *International Journal Quantum Chemistry* **2005**, *103*, 1-9. (*I.F* 1.37)

13. Clark, A. E.[+]; Sonnennberg, J.[#]; Hay, P. J.; Martin, R. L. Density and wave function analysis of actinide complexes: What can fuzzy atom, atoms-in-molecules, Mulliken, Löwdin, and natural population analysis tell us? *Journal of Chemical Physics* **2004**, *121*, 2563-2571. (*I.F* 3.33)

12. Clark, A. E.[#]; Davidson, E. R.; Zaleski, J. M. A TDDFT description of the low-energy excited states of copper and zinc metalloenediynes. *Chemical Communications* **2003**, *23*, 2876-2877. (*I.F* 5.787)

11. Bhattacharyya, S.[+]; Clark, A. E.[#]; Pink, M.; Zaleski, J. M. Isolation of electronic from geometric contributions to Bergman cyclization of metalloenediynes. *Chemical Communications* **2003**, *10*, 1156-1157. (*I.F* 5.787)

10. Clark, A. E.[#]; Davidson, E. R. Population analyses based upon projection operators. *International Journal of Quantum Chemistry* **2003**, *93*, 384-394. (*I.F* 1.37)

9. Clark, A. E.[#]; Davidson, E. R. p-Benzyne derivatives that have exceptionally small singlet-triplet gaps and even a triplet ground state. *Journal of Organic Chemistry* **2003**, *68*, 3387-3396. (*I.F* 4.002)

8. Kraft, B.[#]; Coalter, N. L.[#]; Clark, A. E.[#]; Huffman, J. C.; Zaleski, J. M. Photo-thermally induced cyclization of metalloenediynes via near-infrared ligand-to-metal charge transfer excitation. *Inorganic Chemistry* **2003**, *42*, 1663-1672. (*I.F* 4.326)

7. Davidson, E. R.; Clark, A. E.[#] Model molecular magnets. *Journal of Physical Chemistry A* **2002**, *106,* 7456-7461. (*I.F* 2.732)

6. Clark, A. E.[#]; Davidson, E. R. Local Spin III: Wave function analysis along a reaction coordinate, H atom Abstraction and addition processes of benzyne. *Journal of Physical Chemistry A* **2002**, *106*, 6890-6896. (*I.F* 2.732)

5. Davidson, E. R.; Clark, A. E.[#] Local Spin II. *Molecular Physics* **2002,** *100*, 373-383. (*I.F* 1.743)

4. Clark, A. E.[#]; Davidson, E. R. Model studies of hydrogen-atom abstraction by ortho-, meta-, and para-benzynes. *Journal of the American Chemical Society* **2001**, *123*, 10691-10698. (*I.F* 9.023)

3. Clark, A. E.[#]; Davidson, E. R. Local Spin. *Journal of Chemical Physics* **2001**, *115*, 7382-7393. (*I.F* 3.33)

2. Clark, A. E.[#]; Davidson, E. R.; Zaleski, J. M. UDFT and MCSCF descriptions of the photochemical Bergman cyclization of enediynes. *Journal of the American Chemical Society* **2001**, *123*, 2650-2657. (*I.F* 9.023)

1. Camacho, M. B.[*]; Clark, A. E.[*]; Liebrecht, T.[*]; DeLuca, J. P. A phenyliodonium ylide as a precursor for dicarboethoxycarbene: Demonstration of a strategy for carbene generation. *Journal of the American Chemical Society* **2000**, *122*, 5210-5211. (*I.F* 9.023)

Book Chapters (refereed)

1. Hurst, J. K.; Clark, A. E. Mechanisms of Water Oxidation Catalyzed by Ruthenium Coordination Complexes, *Progress in Inorganic Chemistry*, **2011**, *57*, 1 - 54. (*I.F.* 9.33)
2. Clark, A. E. Intermolecular Network Theory: A General Approach for Understanding the Structural and Dynamic Properties of Liquids and Solutions. In *Annual Reports in Computational Chemistry;* Dixon, D. A., Ed.; **2015**; pp 313–359

Workshop Reports and Conference Proceedings (non-peer reviewed)

DOE BES Basic Research Needs for Environmental Management, Cross-Cutting panel lead (report to be submitted Sept 2015)

DOE Office of Science Workshop on Computational Materials Science and Chemistry for Innovation, Separations and Fluidic Processes panel member. *http://www.ornl.gov/sci/cmsinn/*

DOE BES Basic Research Needs for Advanced Nuclear Energy Systems, Predictive Modeling and Simulation panel member.
http://www.sc.doe.gov/bes/reports/files/ANES_rpt.pdf

Clark, Sue B.; Nash, Ken; Benny, Paul; Clark, Aurora E.; Wall, Nathalie; Wall Don; Yoo, Choon-Shik. Radiochemistry Education at Washington State University: Sustaining Academic Radiochemistry for the Nation, American Institute of Physics Conference Proceedings, **2009**.

Invited Presentations (2009-present)

12/19/2015	International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, HI
7/6/2015	International Conference on Chemical Bonding, Kaui, HI
4/21/2015	DOE BES Contractor meeting, Gaithersberg, MD
4/17/2015	University of California Merced, Department of Chemistry
3/25/2015	Natl. Mtg. American Chemical Society, Design of Materials and Chemical Processes (Phys)
3/5/2015	Reed College, Department of Chemistry
9/15/2014	International Conference on Theoretical and High Performance Computational Chemistry, Academica Sinica, Beijing
9/12/2014	Tsinghua University, Department of Chemistry
9/11/2014	Chinese Academy of Sciences, Beijing, Nuclear Physics Program
9/10/2014	Nanjing University of Technology, Chemical Engineering Department
9/9/2014	Shanghai Institute of Applied Physics
8/11/2014	Natl. mtg. American Chemical Society, Computational Spectroscopy (Phys)
3/20/2014	Natl. mtg. American Chemical Society, Thermodynamics, Reactivity, and Spectroscopy of the Heavy Elements (Phys)
8/28/2013	Goldschmidt 2013, Florence, Italy
12/3/2012	Chemistry Colloquium, University of Oregon
9/25/2012	XVII International Workshop on Quantum Systems in Chemical Physics, Turku Finland
8/20/2012	Natl. mtg. American Chemical Society, Symp. in Honor of Berny Schlegal (Comp)
4/10/2012	Materials Research Society, Actinides – Basic Science and Applications (Y)
3/26/2012	Natl. mtg. American Chemical Society, Symp. in Honor of Lester Morss (Nucl)
8/31/2011	Natl. mtg. American Chemical Society, Symp. Earth Abundant Solar Materials (Inorg)
4/1/2011	DOE BES Contractor meeting, Baltimore, Md
11/15/2010	Chemistry Colloquium, University of Arizona
5/6/2010	Pacific Northwest National Lab
4/16/2010	Chemistry Colloquium, University of North Texas
12/1/2009	Asia Pacific Symposium on Radiochemistry, Napa, CA
11/30/2009	Chemistry Colloquium, University of South. California, Los Angeles, CA

11/2/2009	Chemistry Colloquium, University of Montana, Missoula, MT
9/23/2009	Migration'09, Richland Wa
8/18/2009	Natl. mtg. American Chemical Society, Symposium in Honor of P. Jeffrey Hay (Inorg/DNCT)
6/15/2009	NSF Workshop on Inorganic Chemistry, Park City, UT
5/11/2009	Center for Green Materials Chemistry and Oregon Nanoscience and Microtechnologies Institute
4/15/2009	Quantum Theory Project Colloquium, University of Florida
4/14/2009	Chemistry Colloquium, Florida State University
3/23/2009	Natl. mtg. American Chemical Society, HP Junior Faculty Awards seminar (Comp)
2/24/2009	Argonne National Laboratory, Chemical Sciences and Engineering Division

In the News (most relevant)

- Wired magazine, 2012, "Researchers Fight Toxic Waste With Google PageRank" http://www.wired.com/2012/02/google-pagerank-water/
- Forbes magazine, 2012, "Need to know the structure of a molecule? Google it." http://www.forbes.com/sites/alexknapp/2012/03/06/need-to-know-the-structure-of-a-molecule-google-it/
- The Atlantic, 2012, "A Chemist Uses Google's Algorithm to Determine the Structure of Molecules" http://www.theatlantic.com/technology/archive/2012/02/a-chemist-uses-googles-algorithm-to-determine-the-structure-of-molecules/253151/
- ExtremeTech, 2012, "Applying Google's PageRank Algorithm to the Molecular Universe", http://www.extremetech.com/extreme/118419-applying-googles-pagerank-algorithm-to-the-molecular-universe
- TheVerge, 2012, "Google PageRank Algorithm used in tool to model interactions between molecules", http://www.theverge.com/tag/aurora-clark
- Spokesman Review, 2014, "The Science of Snow", http://www.spokesman.com/picture-stories/science-snow/

Current Funded Projects

Department of Energy 10/1/2015-4/1/2019
Basic Energy Sciences $1,290,000 ($331,530 for A. Clark)
"Development of Approaches to Model Excited-State Charge and Energy Transfer in Solution"
Award #: DE-SC0014437
Role: Co-PI

TerraPower 10/1/2014 – 10/1/2016
"Recycling of used nuclear fuel: An experimental and computational investigation for removal of metal ions of interest using supercritical carbon dioxide systems"
Role: PI (Sue Clark co-PI) $568,624 ($248,638 for A. Clark)

Department of Energy 8/15/2012-8/15/2017
Basic Energy Sciences $7,500,000 ($620,000 for A. Clark)
"Center for Nanoporous Materials Genome for Carbon Capture"

Award #: DE-SC0008688
Role: Co-PI

Department of Energy 12/15/2012 – 12/15/2016
Basic Energy Sciences, Heavy Element Division $410,000
Single Investigator and Small Group Research (SISGR)
"Supramolecular Organization Within Electrolyte Solutions and the Importance of Molecular Hydrophobicity to Successful Actinide Solvent Extraction"
Award #: DE-SC0001815
Role: PI

Previously Funded Projects

Department of Energy 10/15/2011-10/15/2015
Nuclear Energy University Program $500,000
"Rapid Computer Aided Ligand Design and Screening of Precious Metal Extractants from TRUEX Raffinate with Experimental Validation."
Award #: 00014002
Role: PI

Department of Energy 8/1/2009-12/15/2012
Basic Energy Sciences, Heavy Element Division $600,000
Single Investigator and Small Group Research (SISGR)
Origin of Actinide Ion Partitioning in Biphasic Systems
Award #: DE-SC0001815
Role: PI

National Science Foundation 8/15/2009-8/14/2012
CHE SYNTH INORG $200,000
Multiscale Chemistry of U, Np, and Pu Fission Products in Acidic and Basic Media
Award #: 0848346
Role: PI

Department of Energy 4/15/2007-10/15/2010
Nuclear Science, Engineering and Health Physics $225,000
Junior Faculty Award
Classical Simulations of the Aqueous Surface Chemistry of U(VI) Silicates
Award #: DE-FG07-05ID14692
Role: PI

M. J. Murdock Charitable Trust 6/15/2008-8/15/2009
Partners in Science Program $15,000
A Computational Study of the Optical Properties of Organic Dye Aggregates
Role: PI

Courses Taught

Washington State University	Credit Hours
Chemistry 105, Principles of Chemistry I	3

Chemistry 531, Advanced Physical Chemistry I: Thermodynamics	3
Chemistry 331, Physical Chemistry I: Thermodynamics	3
Chemistry 101, Introduction to Chemistry I	4
Chemistry 330, Problem Solving in Physical Chemistry	1
Chemistry 332, Physical Chemistry II: Quantum Mechanics	3
Chemistry 495, Directed Research	1
Chemistry 499, Special Problems in Chemistry	1
Chemistry 532, Advanced Physical Chemistry II: Quantum Mechanics	3
Chemistry 536, Advanced Quantum Chemistry	3
Chemistry 537, Special Topics: Molecular Dynamics	3
Chemistry 537, Special Topics: Applied Computational Chemistry	3
Chemistry 593, Materials Science and Physical Chemistry Seminar	1

Student Training

a. Graduate students and post-doctoral fellows trained in the Clark Laboratory

Name	Dates	Degree	Year
Patrick Pastor	`05-07	MS	`07
Samuel Chen	`06-08	MS	`08
Natalia Zakharova	`08-10	MS	`10
Daniel Sullivan	`11-14	MS	`14
Yasaman Ghadar	`08-14	Ph.D	`14
Alex Samuels	`09-14	Ph.D	`14
Chun-hung Wang	`10-current	Ph.D.	~`15
Morgan Kelley	`11-current	Ph.D	~`15
Tiecheng Zhou	`13-current	Ph.D	~`17
Sujala Bhattarai	'14-current	Ph.D.	~'18
Changyong Qin	`06-07	Post-doc	
Matthew Wander	`07-08	Post-doc	
Jadwiga Kuta	`08-10	Post-doc	
ArunKumar Subramanian	`10-11	Post-doc	
Payal Parmar	`11-current	Post-doc	
Jian Wu	`13-14	Post-doc	
Abdullah Ozkankar	`11-14	Post-doc	
Yasaman Ghadar	`14-current	Post-doc	
Mostafa Kuccukkal	'15 - current	Post-doc	

b. Graduate student committees served

Name	Program	Dates	Degree
Clarissa Carrizales	Chem	2006-2009	MS
Erin Finn	Chem	2006-2008	MS
Harry Zhou	Chem	2006-2009	MS
Krista Nishida	Chem	2005-2010	Ph.D
Ben Friesen	Chem	2005-2010	Ph.D

Stephanie Holbrook	Chem	2008-2009	MS
Talukder Zaki Jubery	MME	2010-2011	MS
David Bross	Chem	2010-2015	Ph.D
James Shearhouse	Chem	2010-2011	MS
Maria Kriz	Chem	2006-2010	Ph.D.
John Hardy	MSEP	2006-2011	Ph.D.
Barbara Mooney	Chemistry – University of Arizona	2007-2012	Ph.D.
John Friederich	Chem	2007-2012	Ph.D.
Fangling Che	ChemE	2012-2016	Ph.D.
Alyssa Hensley	ChemE	2012-2016	Ph.D.
Deborah Malamen	Chem	2012-2014	MS
Rolf Hermanson	Chem	2013-2018	Ph.D.
Qin Lu	Chem	2013-2018	Ph.D.
Chris Leishman	Chem	2013-2017	Ph.D.
Bryan Borders	MSEP	2013-2017	Ph.D.
Cheri Boele	Chem	2012-2014	MS
Adam Burns	Chem	2012-2016	MS
Jeffrey Berry	Chem	2012-2016	Ph.D.
Amber Donley	Chem	2010-2014	Ph.D.