ERIC S. SHAMAY

Contact Information

Department of Chemistry
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Education

University of Oregon, Eugene, OR

PhD, Computational Physical Chemistry, in progress — Expected Mar 2012

Dissertation topic: "Computational modeling and simulation of gaseous adsorption processes on aqueous interfaces"

Advisor: Geraldine L. Richmond

California Polytechnic State University, San Luis Obispo, CA

BS, Chemistry & General Engineering — June 2004

Experience

Richmond Research Group, University of Oregon, Eugene, OR — 8/2005 – present

Graduate Research Assistant

Conducted computational modeling and simulation studies to characterize water's behavior at interfaces between aqueous systems and other phases. Utilized both classical and quantum molecular dynamics techniques, and created a suite of analytical tools, (in C++ and python) for producing computational nonlinear vibrational spectra of water and small inorganic ions and acid species in interfacial environments. Conducted studies on the topologies and geometry of liquid-liquid interfaces and produced visualization tools for the analyses.

Hore Research Group, Univ. of Victoria, B.C. Canada — 1/2008 – 4/2008

Visiting Research Fellow

Visiting researcher in computational chemistry and scientific computing. Modeled aqueous chemical systems of small inorganic salts using classical molecular dynamics simulations. Analyzed the geometries and vibrational spectra of interfacial aqueous environments between salt solutions and an organic carbon tetrachloride phase. The research resulted in publication in the *Jour. of Phys. Chem. C*.

Parrinello Research Group, USI-Campus, Lugano, Switzerland — 11/2006 – 2/2007

IGERT Research Travel Fellowship

Visiting researcher working directly with Dr. Victoria Buch. Simulated aqueous nitric acid interfaces with air/vacuum using quantum molecular dynamics (CP2K/Quickstep). Wrote analytical software (in C++, Fortran) to determine hydration states, the adsorption mechanism, and lifetime of nitric acid near a water surface. Results of the research were published in the *Jour. of Amer. Chem. Soc.*

Channel Islands Opto-Mechanical Engineering, Inc. Ventura, CA — 12/2004 – 6/2005

Engineer and Quality Assurance Manager

Produced a high vacuum coating deposition chamber for gaussian infrared optical filters using electron beam physical vapor deposition techniques. Designed and built an infrared spectrophotometer for coating analysis, and implemented a system for data acquisition (in Labview and C), and designed multiple mechanical subsystems for quality analysis tools (using SolidWorks, ProE). Performed quality control tasks on mechanical systems and optics. Began ISO 9000 certification with creation of a quality control system, manuals, procedures, and forms.

National Institute of Standards and Technology, Gaithersburg, MD — 6/2004 – 8/2004

Undergraduate Research Fellow

Developed a database and web-based front-end for real-fuels combustion models researched at NIST. Produced technologies for polyaromatic hydrocarbon species nomenclature, and substituted hydrocarbon species relational identification (in Perl, Apache, Java, and MySQL). The chemical kinetics toolset is available at *http://kinetics.nist.gov/CKMech.*

Chemistry Dept. California Polytechnic State University, SLO, CA 6/2003 – 6/2004
Research Assistant
Conducted experiments on polyelectrolyte multilayer systems coated on silica substrates. Implemented atomic force microscopy and quartz crystal microgravimetry measurements for surface and polymer deposition characterization. Results were presented at the regional American Chemical Society meeting.

Invensys-Triconex, Irvine, CA 6/2001 – 10/2001
Engineer and Technical Editor
Researched, edited, and produced design requirements for automated fault-insertion system software, and compiled an operations manual. Maintained and updated fault-insertion robotics components. Documented EPROM programming systems to facilitate use of a variety of memory modules.

California Polytechnic State University, SLO, CA 1/2001 – 6/2001
Calpoly Roborodentia Robotics Club Competition
Designed and built a small autonomous maze-solving robot, including a hand-built microprocessor platform (68HC11), custom circuit boards, IR sensors, and stepper motors, and embedded software written in C and assembly language.

Sierra Instruments, Monterey, CA 6/2000 – 9/2000
Engineering Internship
Implemented a Labview front-end for clean-gas data acquisition and mass-flow meter calibration loops. Documented mass-flow calibration procedures and conducted software training. Fulfilled engineering action requests for updating CAD drawings for design changes.

Relevant Coursework

Chemistry: Graduate coursework in thermodynamics (Fermi), kinetics, quantum mechanics (Shankar), statistical mechanics (Chandler), molecular spectroscopy (McHale). Undergraduate coursework in quantum mechanics, instrumental analysis, quantitative analysis, organic chemistry (McMurry). **Engineering**: undergraduate coursework in mechanical control systems (Nise), mechanical vibrations (Steidel), acoustics, thermodynamics, engineering dynamics, fluid mechanics (McDonald), computer organization (P&H), heat transfer (Dewitt), data structures & algorithms (Cormen & L,R,S).

Selected Publications

Shamay, E. and G.L. Richmond. "Ionic disruption of the liquid-liquid interface." *Jour. of Phys. Chem. C*, Vol. 114, Iss. 29, (Jul 29 2010) pp. 12590-12597.

Shamay, E. and G.L. Richmond. "Interfacial aqueous solution structure near surfaces of organic fluids and hydrophobic monolayers." *239th ACS national meeting,* San Francisco, March 2010.

Kido Soule, M. and P.G. Blower, **E. Shamay**, G.L. Richmond. "How nitric acid changed my life: At the edge of computational simulation and nonlinear vibrational spectroscopy." *Materials Science Institute / IGERT retreat,* Dec 2007.

Shamay E. and V. Buch, M Parrinello, G.L. Richmond. "At the water's edge: Nitric acid as a weak acid." *Jour. of the American Chem. Soc.*, Vol. 129, Iss. 43, (Oct 31 2007) pp 12910-+.

Shamay, E. and R. Grant, D.E. Gragson. "Polyelectrolyte multilayer film morphology and water adsorption explored by atomic force microscopy and quartz crystal microgravimetry." *227th ACS national meeting*, Anaheim, March 2004.

Skills

Expert C++ programmer and UNIX user.

Proficient in C, Python, STL and Boost libraries, parallel computing algorithms.

Previous experience with LabView, Common Lisp, Haskell, Perl.

Basic analog and digital electronic circuit design and construction.

Proficient with use of various CAD packages for mechanical drafting and design.

Extensive knowledge of computational molecular simulation techniques and software.

System administration of a small academic computing cluster.

Experienced with chemical synthesis and analytical techniques.

Native Hebrew language speaker.