ERIC SCHWEGLER

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Education

Ph.D. Physical Chemistry, University of Minnesota, Minneapolis, MN 1998
Thesis: *Linear scaling computation of the Hartree-Fock exchange matrix*
Advisors: Prof. Donald G. Truhlar and Dr. Matt Challacombe

B.S. Chemistry and Computer Science, Southwestern University, TX 1991

Professional Appointments and Leadership Positions

Group Leader, Lawrence Livermore National Laboratory 2005-present

Lead and manage the Quantum Simulations Group (QSG), which currently consists of 16 staff members, 6 postdocs and 2 graduate students (www.llnl.gov/qsg). The QSG specializes in combining state-of-the-art quantum simulation approaches with large-scale computing to validate, understand and predict the properties of materials that are relevant to the national security missions of LLNL. The current major research areas within the QSG include the development and use of quantum simulations to determine the equation of state of materials under extreme conditions, the discovery and optimization of materials for energy technologies, the construction of realistic materials models for applications such as radiation detection, quantum computing, and optical materials, and the continual development of advanced theoretical models for electronic structure.

Leadership Team, Critical Materials Institute (CMI) 2013-present

Serve as the Crosscutting Research Focus Area Lead within CMI, a DOE Energy Innovation Hub. Responsible for coordinating the research being carried out at eight different institutions over three main research thrusts, including Enabling Science, Environmental Sustainability, and Supply Chain & Economic Analysis. LLNL point of contact for CMI.

Lab Program Coordinator, Basic Energy Sciences (BES) 2013-present

Responsible for overseeing the portfolio of BES supported research at LLNL. Interact directly with BES staff to manage the core LLNL projects, develop new science initiatives and serve as the primary point of contact and interface to the BES MSE, SUF, and CSGB Divisions.

Educational Outreach, CCMS and NNSA/MSIPP 2002-present

Primary organizer and director for the Computational Chemistry and Materials Sciences (CCMS) Summer Institute program (www.llnl.gov/ccms) and participant in the NNSA Minority Serving Institution Partnership Program (MSIPP). Started in 2002, the CCMS program enables 10-20 graduate students each summer to work directly with LLNL scientists on the application of cutting-edge methods in computational materials science and chemistry and attend a series of mini-courses given by leading external experts. Since 2013, the CCMS has been included as a component of the NNSA/MSIPP consortium at

LLNL and has hosted students and faculty from Florida A&M University, Tuskegee and Prairie View A&M University.

Staff Physicist, Lawrence Livermore National Laboratory 2001-2005
Principal investigator for the ASC/PEM Advanced Equation of State program. Developed and implemented a plan for the construction of highly accurate equation of state tables based on quantum simulations based approaches. Carried out a systematic examination of the accuracy that can be achieved in ab initio molecular dynamics simulations of liquids such as water and systematically examined how the properties of fluids are changed in highly confined spaces at the nanoscale.

Postdoctoral Researcher, Lawrence Livermore National Laboratory 1998-2001
Developed and applied new computational approaches for mapping out a materials phase boundaries under high temperature and pressure conditions. In particular, the two-phase coexistence approach for determining melting curves was implemented in a first-principles context for the first time and demonstrated on materials of programmatic interest.

Honors and Awards

Fellow of the American Physical Society – 2013
NNSA Defense Programs Award of Excellence – 2013
Outstanding Postdoc Mentor Award – 2010
Department of Energy INCITE Award – 2007, 2008
LLNL Science and Technology Award – 2006
National Ignition Facility Program Award – 2006
Physics and Advanced Technologies Directorate Awards – 2002, 2003, 2005

LLNL Institutional Activities

Basic Energy Science Program Coordinator for LLNL, 2013-present
Materials for Energy APL, Global Security, 2014-present
Director of the Computational Chemistry and Materials Science (CCMS) Summer Institute
Institutional Computing Executive Group member, 2005-present
Lawrence Fellowship Selection Committee, 2008-present

Conference Organization

Organizer of the Earth and Planetary Materials Focus Session at the 2006 APS March meeting
Organizer of the Computational Nanoscience Focus Session at the 2007 APS March meeting
Organizer of the Weak Interactions Phenomena Session at the 2008 MRS Spring meeting
Program Committee Member for DCOMP at the 2010 APS March meeting
Technical Committee Member for the 2013 APSSCCM/AIRAPT Joint Conference

Publications (>4400 citations, h-index=31)

A. Goliaei, E.Y. Lau, U. Adhikari, E. Schwegler, M.L. Berkowitz "Behavior of P85 and P188 Poloxamer Molecules: Computer Simulations Using United-Atom Force-Field", *Journal of Physical Chemistry B* in press (2016).

A. Samanta, M. Morales, E. Schwegler "Exploring the free energy surface using ab initio molecular dynamics", *Journal of Chemical Physics* 144, 164101 (2016).

T.A. Pham, G. Mortuza, B. Wood, E. Lau, T. Ogitsu, S. Bushsbaum, Z. Siwy, F. Fornasiero, E. Schwegler "Salt Solutions in Carbon Nanotubes: The Role of Cation-pi Interactions", *Journal of Physical Chemistry C*, 120, 7332 (2016).

E. Lau, M.L. Berkowitz, E. Schwegler "Shock Wave-Induced Damage of a Protein by Void Collapse", *Biophysical Journal* **110**, 147 (2016).

W.I. Choi, B.C. Wood, E. Schwegler, T. Ogitsu "Combinatorial Search for High-Activity Hydrogen Catalysts Based on Transition-Metal-Embedded Graphitic Carbons", *Advanced Energy Materials* **5**, 1501423 (2015).

T.A. Pham, D. Lee, E. Schwegler, G. Galli "Interfacial effects on the band edges of functionalized Si surfaces in liquid water", *Journal of the American Chemical Society* **136**, 17071 (2014).

L.X. Benedict, K.P. Driver, S. Hamel, B. Militzer, T.T. Qi, A.A. Correa, A. Saul, E. Schwegler "Multiphase equation of state for carbon addressing high pressures and temperatures" *Physical Review B* **89**, 224109 (2014).

P. Huang, T.A. Pham, G. Galli, E. Schwegler "Alumina(0001)/Water Interface: Structural Properties and Infrared Spectra from First-Principles Molecular Dynamics Simulations" *Journal of Physical Chemistry C* **118**, 8944 (2014).

D. Lee, E. Schwegler, Y. Kanai "Dependence of water dynamics on molecular adsorbates near hydrophobic surfaces: First principles molecular dynamics study" *Journal of Physical Chemistry C* **118**, 8508 (2014).

T.A. Pham, C. Zhang, E. Schwegler, G. Galli "Probing the electronic structure of water with many-body perturbation theory" *Physical Review B* **89**, 060202 (2014).

B.C. Wood, E. Schwegler, W.I. Choi, T. Ogitsu "Surface chemistry of GaP(001) and InP(001) in contact with water" *Journal of Physical Chemistry C* **118**, 1062 (2014).

W.I. Choi, B.C. Wood, E. Schwegler, T. Ogitsu "Site-dependent free energy barrier for proton reduction on MoS2 edges" *Journal of Physical Chemistry C* **117**, 21772 (2013).

B.C. Wood, E. Schwegler, W. I. Choi, T. Ogitsu "Hydrogen-bond dynamics of water at the interface with InP/GaP(001) and its implications for photoelectrochemistry" *Journal of the American Chemical Society*, **135**, 15774 (2013).

M. M. Morales, S. Hamel, K. Caspersen, E. Schwegler "Hydrogen-helium demixing from first principles: From diamond anvil cells to planetary interiors" *Physical Review B* **87**, 174105 (2013)

T. Ogitsu, E. Schwegler, G. Galli "β-rhombohedral boron: At the crossroads of the chemistry of boron and the physics of frustration" *Chemical Reviews*, **113**, 3425 (2013)

T. Ogitsu, E. Schwegler "The alpha-beta phase boundary of elemental boron" *Solid State Sciences* **14**, 1598 (2012)

Hamel, S. *et al*. "Equation of state of $CH_{1.36}$: First-principles molecular dynamics simulations and shock-and-release wave speed measurements" *Physical Review B* **86**, 094113 (2012)

T.A. Pham, P. Huang, E. Schwegler, G. Galli "First-Principles Study of the Infrared Spectra of the Ice Ih (0001) Surface" *Journal of Physical Chemistry A* **116**, 9255 (2012)

H.J. Kulik, E. Schwegler, G. Galli "Probing the Structure od Salt Water under Confinement with First-Principles Molecular Dynamics and Theoretical X-ray Absorption Spectroscopy" *Journal of Physical Chemistry Letters* **3**, 2653 (2012)

T. Ogitsu, *et al.* "Ballistic electron transport in non-equilibrium warm dense gold" *High Energy Density Physics* **8**, 303 (2012)

J.R.I. Lee, *et al.* "Ligand-Mediated Modification of the Electronic Structure of CdSe Quantum Dots" *Nano Letters* **12**, 2763 (2012)

J. Kang, J. Zhu, S.H. Wei, E. Schwegler, Y.H. Kim "Persistent medium-range order and anomalous liquid properties of $Al_{1-x}Cu_x$ alloys" *Physical Review Letters* **108**, 115901 (2012)

B.C. Wood, T. Ogitsu, E. Schwegler "Local structural models of complex oxygen- and hydroxyl-rich GaP/InP(001) surfaces" *Journal of Chemical Physics* **136**, 064705 (2012)

M.A. Morales, LX. Benedict, D.S. Clark, E. Schwegler, I. Tamblyn, S.A. Bonev, A.A. Correa, S.W. Haan "Ab initio calculations of the equation of state of hydrogen in a regime relevant for intertial fusion applications", *High Energy Density Physics* **8**, 5 (2012)

D.C. Swift, J.H. Eggert, G.G. Kicks, S. Hamel, K. Caspersen, E. Schwegler, G.W. Collins, N. Nettlemann, G.J. Ackland "Mass-radius relationships for exoplanets", *Astrophysical Journal* **744**, 59 (2012)

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B.C. Wood, T. Ogitsu, E. Schwegler "Ab initio modeling of water-semiconductor interfaces for photocatalytic water splitting: role of surface oxygen and hydroxyl" *Journal of Photonics for Energy* **1**, 016002 (2011)

L. Spanu, D. Donadio, D. Hohl, E. Schwegler, G. Galli "Stability of hydrocarbons at deep Earth pressures and temperatures", *Proceedings of the National Academy of Sciences* 108, 6843 (2011)

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Y. Ping, A.A. Correa, T. Ogitsu, E. Draeger, E. Schwegler, T. Ao, K. Widmann, D.F. Price. E. Lee, H. Tam, P.T. Springer, D. Hanson, I. Koslow, D. Prendergast, G. Collins, A. Ng, "Warm dense matter created by isochoric laser heating", *High Energy Density Physics* **6**, 246 (2010)

H. Kulik, N. Marzari, A.A. Correa, D. Prendergast, E. Schwegler, G. Galli, "Local effects in the X-ray absorption spectrum of salt water", *Journal of Physical Chemistry B* **114**, 9594 (2010)

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Eric Schwegler, Manu Sharma, François Gygi and Giulia Galli, "Melting of water under pressure", *Proceedings of the National Academy of Sciences* **105**, 14779 (2008)

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Giancarlo Cicero, Jeffrey C. Grossman, Eric Schwegler, François Gygi and Giulia Galli, "Water confined in nanotubes and between graphene sheets: A first principle study", *Journal of the American Chemical Society* **130**, 1871 (2008)

Markus Allesch, Felice C. Lightstone, Eric Schwegler and Giulia Galli, "First principles and classical molecular dynamics simulations of solvated benzene", *Journal of Chemical Physics* **128**, 014501 (2008)

Jean-Yves Raty, Eric Schwegler, Stanimir A. Bonev, "Electronic and structural transitions in dense liquid sodium", *Nature* **449**, 448 (2007)

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Daniel Orlikowski, Alfredo A. Correa, Eric Schwegler and John E. Klepeis "A Steinberg-Guinan model for high-pressure carbon: diamond phase", *AIP Conference Proceedings* **955**, 247 (2007)

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Jun Fu Lin, Eric Schwegler and Choong-Shik Yoo "Phase Diagram and Physical Properties of H_2O at High Pressures and Temperatures: Applications to Planetary Interiors", Earth's Deep Water Cycle, Geophysical Monograph Series **168**, 159 (2006)

C.J. Tymzak, Valery T. Weber, Eric Schwegler and Matt Challacombe "Linear scaling computation of the Fock matrix. VIII. Periodic boundaries for exact exchange at the Gamma point", *Journal of Chemical Physics* **112**, 124105 (2005)

Felice C. Lightstone, Eric Schwegler, Markus Allesch, François Gygi and Giulia Galli "A first-principles molecular dynamics study of calcium in water", *ChemPhysChem* **6**, 1745 (2005)

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Eric Schwegler, Jeffrey C. Grossman, François Gygi and Giulia Galli "Towards an assessment of the accuracy of density functional theory for first principles simulations of water II", *Journal of Chemical Physics* **121**, 5400 (2004)

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Fernando A. Reboredo, Eric Schwegler, and Giulia Galli "Optically Activated Functionalization Reactions in Si Quantum Dots" *The Journal of the American Chemical Society* **125**, 15243 (2003)

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Eric Schwegler, Giulia Galli, and François Gygi "Conformational dynamics of the dimethyl phosphate anion in solution", *Chemical Physics Letters* **342**, 434 (2001)

Jody White, Eric Schwegler, Giulia Galli, and François Gygi "Solvation of Na+ in water: first principles molecular dynamics", *Journal of Chemical Physics* **113**, 4668 (2000)

Eric Schwegler, Giulia Galli, and François Gygi “Water under pressure”, *Physical Review Letters* **84**, 2429 (2000)

Eric Schwegler and Matt Challacombe “Linear scaling computation of the Fock matrix. III. Formation of the exchange matrix with permutational symmetry”, *Theoretical Chemistry Accounts* **104**, 344 (2000)

Eric Schwegler and Matt Challacombe “Linear scaling computation of the Fock matrix. IV. Multipole accelerated formation of the exchange matrix”, *Journal of Chemical Physics* **111**, 6223 (1999)

Eric Schwegler, Matt Challacombe, and Martin Head-Gordon “Multipole acceptability criteria for electronic structure theory”, *Journal of Chemical Physics* **109**, 8764 (1998)

Eric Schwegler, Matt Challacombe, and Martin Head-Gordon “Linear scaling computation of the Fock matrix. II. Rigorous bounds on exchange integrals and incremental Fock builds”, *Journal of Chemical Physics* **106**, 9703 (1997)

Matt Challacombe and Eric Schwegler “Linear scaling computation of the Fock matrix”, *Journal of Chemical Physics* **106**, 5526 (1997)

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Eric Schwegler, Pawel Kozlowski, and Ludwik Adamowicz “Applications of explicitly correlated Gaussian-type functions for the ground state of the beryllium atom”, *Journal of Computational Chemistry* **14**, 566 (1993)