Ross Eliot Larsen

National Renewable Energy Laboratory
Computational Science Center
Email: therosslarsen@gmail.com Phone: (805)452-2042

EDUCATION

Brown University, Providence, RI (1993-1998)
Sc.M., Physics, 1996
Ph.D., Physics, 1998
Thesis: "Static and Dynamic Properties of Molecules Dissolved in Liquids"
Advisor: Richard M. Stratt

University of Puget Sound, Tacoma, WA (1989-1993)
B.S., Honors in Physics, 1993

RESEARCH EXPERIENCE

Fellow Renewable and Sustainable Energy Institute, CU Boulder (2020–)

Senior Scientist National Renewable Energy Laboratory (2009–)
Computational Science Center
Scientist V (2013–)
Scientist IV (2009–2013)

Staff Scientist (2006–2009)/**Postdoctoral Fellow** (2001-2006)
University of California at Los Angeles
Advisor: Benjamin J. Schwartz
Mixed quantum/classical molecular dynamics of solvent-supported electronic states

Postdoctoral Fellow: University of California at Santa Barbara (1998–2001)
Advisor: Horia Metiu
Spatial resolution and polarization in apertureless near-field microscopy

Research Assistant: Brown University (1994–1998)
Advisor: Richard M. Stratt

Research Assistant: University of Puget Sound (1992–93)
Murdock Charitable Trust Award
Advisor: Andrew F. Rex

Research Assistant: University of Puget Sound (1991)
Advisor: Alan S. Thorndike

TEACHING EXPERIENCE

Lecturer: UCLA Department of Chemistry and Biochemistry (2007–2009)
Chemistry 14A (Winter '09): Atomic and Molecular Structure, Equilibria, Acids and Bases
Chemistry 110A (Spring '08): Chemical Thermodynamics
Chemistry 14A (Winter '08): Atomic and Molecular Structure, Equilibria, Acids and Bases
Chemistry 20A (Summer '07): Chemical Structure

Teaching Assistant: Brown University Physics Department (1993–1994)

Teaching Assistant: University of Puget Sound Physics Department (1990–1993)

Teaching Assistant: Summer School Mathematics (1990)
Bellevue Public Schools, Bellevue, WA.

PROFESSIONAL SERVICE AND ACTIVITIES

NREL Mentor for multiple DOE Computational Science Graduate Fellows and a NASA Graduate Fellow.

Reviewer for *The Journal of Chemical Physics*, *The Journal of Physical Chemistry*, *Physical Chemistry Chemical Physics* and other journals

Proposal reviewer for multiple U.S. Department of Energy programs

Organizer, UCLA *CNSI NanoHour* seminar series, 2004–2005

Member of American Chemical Society, 2004–

HONORS AND AWARDS

Alliance for Sustainable Energy Chairman's Award for Exceptional Performance, 2013

University of California at Los Angeles California Nanosystems Institute (2004–2005): CNSI/Hewlett–Packard Postdoctoral Fellowship

NSF Travel Award, CECAM Workshop on INM, 1999.

Brown University Potter Prize for Outstanding Dissertation in Chemistry, 1998.

Brown University Research Fellowship, 1998.

University of Puget Sound Seward Scholar, academic years 1991–1992 and 1992–1993.

University of Puget Sound Trustee Scholar, 1989–1993.

PUBLICATIONS

58. M.-A. Ha and R. E. Larsen, "Multiple Reaction Pathways for the Oxygen Evolution Reaction May Contribute to IrO2 (110)'s High Activity", *J. Electrochem. Soc.*, **168**, 024506 (2021).

57. X. He, R. E. Larsen, Z. Y. Shou, F. L. Chen, H. M. Yin, "Block Cracking in Surface Coatings of Polymeric Substrates", *Eng. Fract. Mech.*, **233**, 107073 (2020).

56. A. M. Alia, M.-A. Ha, G. C. Anderson, C. Ngo, S. Pylypenko, and R. E. Larsen, "The Roles of Oxide Growth and Sub-Surface Facets in Oxygen Evolution Activity of Iridium and Its Impact on Electrolysis." *J. Electrochem. Soc.*, **10**, F1243 (2019).

55. K. E. Watts, T. Nguyen, B. J. Tremolet de Villers, B. Neelamraju, M. A. Anderson, W. A. Braunecker, A. J. Ferguson, R. E. Larsen, B. W. Larson, Z. R. Owczarczyk, J. R. Pfeilsticker, J. E. Pemberton, E. L. Ratcliff, "Stability of push-pull small molecule donors for organic photovoltaics: spectroscopic degradation of acceptor endcaps on benzo[1,2-b: 4,5-b']dithiophene core", *J. Mat. Chem. A*, **7**, 19984-19995 (2019).

54. P. C. St. John, C. Phillips, T. W. Kemper, A. N. Wilson, M. F. Crowley, M. R. Nimlos, R. E. Larsen, "Message-passing neural networks for high-throughput polymer screening", *J. Chem. Phys.*, **150**, 234111 (2019).

53. X. He, R. E. Larsen, F. L. Chen, H. M. Yin, "Residual Stress and Opening-Mode Fracture Analysis of Multilayered Structures Subjected to Thermal Loading ", *J. Eng. Mech.* **145**, 04019010 (2019).

52. X. He, R. Tirawat, and R. E. Larsen, (2018) "The Effect of Aging on the Delamination Fracture Energy of Glass Solar Reflectors", CO: National Renewable Energy Laboratory. NREL/TP-2C00-72309. https://www.nrel.gov/docs/fy18osti/72309.pdf

51. M. M. Henry, M. L. Jones, S. D. Oosterhout, T. .W. Kemper, R. E. Larsen, N. Kopidakis, M. F. Toney, D. C. Olson, and E. Jankowski, "Simplified models for accelerated structural prediction of conjugated polymers for organic photovoltaics", *J. Phys. Chem. C*, **121**, 26528-26538 (2017).

50. C. Zhang, F. Chen, M. H. Gray, R. Tirawat and R. E. Larsen, "An elasto-plastic solution for channel cracking of brittle coating on polymer substrate", *International Journal of Solids and Structures*, **120**, 125-136 (2017).

49. K. M. Pelzer, Á. Vázquez-Mayagoitia, L. E. Ratcliff, S. Tretiak, R. A. Bair, S. K. Gray, T. Van Voorhis, R. E. Larsen, S. B. Darling, "Molecular Dynamics and Charge Transport in Organic Semiconductors: A Classical Approach to Modeling Electron Transfer", *Chem. Sci.*, **8**, 2597-2609 (2017).

48. T. W. Kemper, T. Gennett, R. E. Larsen, "Molecular dynamics simulation study of solvent and state of charge effects on solid phase structure and counterion binding in a nitroxide-radical containing polymer energy storage material", *J. Phys. Chem. C*, **120**, 25639-25646 (2016).

47. R. E. Larsen, "Simple Extrapolation Method to Predict the Electronic Structure of Conjugated Polymers from Calculations on Oligomers", *J. Phys. Chem. C*, **120**, 9650-9660 (2016).

46. T. W. Kemper, R. E. Larsen, T. Gennett, "Density of States and the Role of Energetic Disorder in Charge Transport in an Organic Radical Polymer in the Solid State", *J. Phys. Chem. C*, **119**, 21369-21375 (2015).

45. S. D. Oosterhout, N. Kopidakis, Z. R. Owczarczyk, W. A. Braunecker, R. E. Larsen, E. R. Ratcliff, D. C. Olson, "Integrating Theory, Synthesis, Spectroscopy and Device Efficiency to Design Donor Materials for Organic Photovoltaics: A Case Study Including 12 Donors", *J. Mater. Chem. A*, **3**, 9777-9788 (2015).

44. C. Zhang, N. Waksmanski, V. M. Wheeler, E. Pan, R. E. Larsen, "The effect of photodegradation on effective properties of polymeric thin films: A micromechanical homogenization approach", *Int. J. of Eng. Sci.*, **94**, 1-22 (2015).

43. D. C. Bobela, B. K. Hughes, W. A. Braunecker, R. E. Larsen, and T. Gennett, "Close Packing of Nitroxide Radicals in Stable Organic Radical Polymeric Materials", *J. Phys. Chem. Lett.*, **6**, 1414-1419 (2015).

42. B. K. Hughes, W. A. Braunecker, A. J. Ferguson, T. W. Kemper, R. E. Larsen, T. Gennett, "Quenching of the perylene fluorophores by stable nitroxide radical-containing macromolecules", *J. Phys. Chem. B*, **118** 12541 (2014).

41. T. W. Kemper, R. E. Larsen, T. Gennett, "Relationship between molecular structure and electron transfer in a nitroxyl-radical polymer energy storage material", *J. Phys. Chem. C*, **118** 17213 (2014).

40. Z. R. Owczarczyk, W. A. Braunecker, S. D. Oosterhout, N. Kopidakis, R. E. Larsen, D. S. Ginley, D. C. Olson, "Cyclopenta[c]thiophene-4,6-dione-b organic photovoltaic donor materials", *Adv. En. Mat.*, 1301821 (2014).

39. W. A. Braunecker, S. D. Oosterhout, Z. R. Owczarczyk, R. E. Larsen, N. Kopidakis, D. S. Ginley, B. W. Larson, O. V. Boltalina, S. H. Strauss, D. C. Olson, "Ethynylene-linked donor-acceptor alternating copolymers", *Macromol.*, **46**, 3367 (2013).

38. Z. R. Owczarczyk, W. A. Braunecker, A. Garcia, R. E. Larsen, A. M. Nardes, N. Kopidakis, D. S. Ginley, D. C. Olson,"5,10-Dihydroindolo[3,2-b]indole-Based Copolymers with Alternating Donor and Acceptor Moieties for Organic Photovoltaics", *Macromol.*, **46**, 1350 (2013).

37. J. R. Casey, R. E. Larsen, and B. J. Schwartz, "Resonance Raman and temperature-dependent electronic absorption spectra of cavity and noncavity models of the hydrated electron", *Proc. Nat. Acad. Sci.*, **110**, 2712 (2013).

36. W. A. Braunecker, Z. R. Owczarczyk, A. Garcia, N. Kopdakis, R. E. Larsen, S. Hammond, D. S. Ginley, and D. C. Olson, "Benzodithiophene and Imide-Based Copolymers for Photovoltaic Applications", *Chem. Mat.*, **24**, 1346 (2012).

35. A. M. Nardes, A. J. Ferguson, J. B. Whitaker, B. W. Larson, R. E. Larsen, K. Maturová, P. A. Graf, O. V. Boltalina, S. H. Strauss, N. Kopidakis "Beyond PCBM: Understanding the photovoltaic performance of blends of indene-C60 multiadducts with poly(3-hexylthiophene)" *Adv. Func. Mat.*, **22**, 4115 (2012).

34. W. J. Glover, R. E. Larsen, and B. J. Schwartz, "Simulating the formation of sodium:electron tight contact pairs: Watching the solvation of atoms in liquids one molecule at a time", *J. Phys. Chem. A*, **115**, 5887 (2011).

33. R. E. Larsen, W. J. Glover, and B. J. Schwartz, "Response to Comments on *'Does the hydrated electron occupy a cavity?'* " *Science* **331**, 1387 (2011).

32. M. O Reese, A. M. Nardes, B. L. Rupert, R. E. Larsen, D. C. Olson, M. T. Lloyd, S. E. Shaheen, D. S. Ginley, G. Rumbles, and N. Kopidakis, "Photoinduced degradation mechanisms in polymer and polymer-fullerene active layers: Experiment and theory," *Adv. Func. Mat.*, **20**, 3476 (2010).

31. W. J. Glover, R. E. Larsen, and B. J. Schwartz, "The nature of sodium atoms/(Na^+, e^-) contact pairs in liquid tetrahydrofuran," *J. Phys. Chem. B*, **114**, 11535 (2010).

30. R. E. Larsen, W. J. Glover, and B. J. Schwartz, "Does the hydrated electron occupy a cavity?," *Science* **329**, 65 (2010).

29. W. J. Glover, R. E. Larsen, and B. J. Schwartz, "First principles multi-electron mixed quantum classical simulations in the condensed phase II: The charge-transfer-to-solvent states of sodium anions in liquid tetrahydrofuran", *J. Chem. Phys.*, **132**, 144102 (2010).

28. W. J. Glover, R. E. Larsen, and B. J. Schwartz, "First principles multi-electron mixed quantum classical simulations in the condensed phase I: An efficient Fourier grid method for solving the many-electron problem", *J. Chem. Phys.*, **132**, 144101 (2010).

27. W. J. Glover, R. E. Larsen, and B. J. Schwartz, "How does a solvent affect chemical bonds? Mixed quantum/classical simulations of chemical bond dynamics with a full CI treatment of the bonding electrons," *J. Phys. Chem. Lett.***1**, 165 (2010).

26. R. E. Larsen, W. J. Glover, and B. J. Schwartz, "Comment on "An electron-water pseudopotential for condensed phase simulation [J. Chem. Phys. **86**,3462 (1987)," *J. Chem. Phys.*, **131**, 037101 (2009).

25. R. E. Taylor, C. T. Carver, R. E. Larsen, S. Bai, O. Dmitrenko, and C. Dybowski, "Revisiting $HgCl_2$: A Solution and Solid-State ^{199}Hg NMR and ZORA-DFT Computational Study," *J. Mol. Struct.* **930**, 99 (2009).

24. W. J. Glover, R. E. Larsen and B. J. Schwartz, "The Roles of Electronic Exchange and Correlation in Charge-transfer-to-solvent Dynamics: Many-electron Non-adiabatic Mixed Quantum/Classical Simulations of Photoexcited Sodium Anions in the Condensed Phase," *J. Chem. Phys.*, **129**, 164505 (2008).

23. I. A. Shkrob, W. J. Glover, R. E. Larsen, and B. J. Schwartz, "The Structure of the Hydrated Electron. II. A Mixed Quantum/Classical Molecular Dynamics/ Embedded–Cluster Density Functional Theory Study", *J. Phys. Chem. A*, **111**, 5232 (2007).

22. M. C. Cavanagh, R. E. Larsen, and B. J. Schwartz, "Watching Na Atoms Solvate into Na^+:e^- Contact Pairs: Untangling the Ultrafast Charge–Transfer–to–Solvent Dynamics of Na^- in Tetrahydrofuran (THF)", *J. Phys. Chem. A*, **111**, 5144 (2007).

21. M. J. Bedard–Hearn, R. E. Larsen, and B. J. Schwartz, "Moving Solvated Electrons with Light: Nonadiabatic Mixed Quantum/Classical Molecular Dynamics Simulations of the Relocalization of Photoexcited Solvated Electrons in Tetrahydrofuran (THF)", *J. Chem. Phys.*, **125**, 194509 (2006).

20. R. E. Larsen, M. J. Bedard–Hearn, and B. J. Schwartz, "Exploring the Role of Decoherence in Condensed–Phase Nondiabatic Dynamics: A Comparison of Different Mixed Quantum/Classical Simulation Algorithms for the Excited Hydrated Electron", *J. Phys. Chem. B*, **110**, 20055 (2006).

19. M. J. Bedard–Hearn, R. E. Larsen, and B. J. Schwartz, "Projections of Quantum Observables onto Classical Degrees of Freedom in Mixed Quantum–Classical Simulations: Understanding Linear Response Failure for the Photoexcited Hydrated Electron", *Phys. Rev. Lett.***97**, 130403 (2006).

18. C. J. Smallwood, C. N. Mejia, W. J. Glover, R. E. Larsen, and B. J. Schwartz, "A Computationally Efficient Exact Pseudopotential Method. II. Application to the Molecular Pseudopotential of Tetrahydrofuran (THF) with an Excess Electron", *J. Chem. Phys.*, **125**, 074103 (2006).

17. C. J. Smallwood, R. E. Larsen, W. J. Glover, and B. J. Schwartz, "A Computationally Efficient Exact Pseudopotential Method. I. Analytic Reformulation of the Phillips–Kleinman Theory", *J. Chem. Phys.*, **125**, 074102 (2006).

16. R. E. Larsen and B. J. Schwartz, "Nonadiabatic Molecular Dynamics Simulations of Correlated Electrons in Solution. 2. A Prediction for the Observation of Hydrated Dielectrons with Pump–probe Spectroscopy", *J. Phys. Chem. B*, **110**, 9692 (2006).

15. R. E. Larsen and B. J. Schwartz, "Nonadiabatic Molecular Dynamics Simulations of Correlated Electrons in Solution. 1. Full Configuration–Interaction (CI) Excited–state Relaxation Dynamics of Hydrated Dielectrons", *J. Phys. Chem. B*, **110**, 9681 (2006).

14. R. E. Larsen and B. J. Schwartz, "Full Configuration–Interaction Computer Simulation Study of the Thermodynamic and Kinetic Stability of Hydrated Dielectrons", *J. Phys. Chem. B*, **110**, 1006 (2006).

13. M. J. Bedard–Hearn, R. E. Larsen, and B. J. Schwartz, "Mean–field Dynamics with Stochastic Decoherence (MF–SD): A New Algorithm for Nonadiabatic Mixed Quantum/Classical Molecular Dynamics Simulations with Nuclear–Induced Decoherence", *J. Chem. Phys.*, **123**, 234106 (2005).

12. M. J. Bedard–Hearn, R. E. Larsen, and B. J. Schwartz, "The Role of Solvent Structure in the Absorption Spectrum of Solvated Electrons: Mixed Quantum/Classical Simulations in Tetrahydrofuran", *J. Chem. Phys.*, **122**, 134506 (2005).

11. R. E. Larsen and B. J. Schwartz, "Mixed Quantum/Classical Molecular Dynamics Simulations of the Hydrated Dielectron: The Role of Exchange in Condensed–Phase Structure, Dynamics and Spectroscopy", *J. Phys. Chem. B*, **108**, 11760 (2004).

10. M. J. Bedard–Hearn, R. E. Larsen and B. J. Schwartz, "Understanding Nonequilibrium Solute and Solvent Motions Through Molecular Projections: Computer Simulations of Solvation Dynamics in Liquid Tetrahydrofuran (THF)", *J. Phys. Chem. B*, **107**, 14464 (2003).

9. C. J. Smallwood, W. B. Bosma, R. E. Larsen, and B. J. Schwartz, "The Role of Electronic Symmetry in Charge–Transfer–to–solvent (CTTS) Reactions: Quantum Non–Adiabatic Computer Simulation of Photoexcited Sodium Anions", *J. Chem. Phys.*, **119**, 11263 (2003).

8. R. E. Larsen and B. J. Schwartz, "Efficient Real-space Configuration-Interaction Method for Simulation of Multi-Electron Mixed Quantum/Classical Non-Adiabatic Molecular Dynamics in the Condensed Phase", *J. Chem. Phys.*, **119**, 7672 (2003).

7. M. J. Bedard-Hearn, R. E. Larsen, and B. J. Schwartz, "Hidden Breakdown of Linear Response: Projections of Molecular Motions in Nonequilibrium Calculations of Solvation Dynamics", *J. Phys. Chem. A*, **107**, 4773 (2003).

6. R. E. Larsen and H. Metiu, "Resolution and Polarization in Apertureless Near-Field Microscopy", *J. Chem. Phys.*, **114**, 6851 (2001).

5. R. E. Larsen and R. M. Stratt, "Instantaneous Pair Theory for High-Frequency Vibrational Energy Relaxation in Fluids", *J. Chem. Phys.*, **110**, 1036 (1999).

4. R. E. Larsen and R. M. Stratt, "Mutual-nearest-neighbor pairs in fluids", *Chem. Phys. Lett.*, **297**, 211 (1998).

3. R. E. Larsen, E. F. David, G. Goodyear, and R. M. Stratt, "Instantaneous Perspectives on Solute Relaxation in Fluids: The Common Origins of Nonpolar Solvation Dynamics and Vibrational Population Relaxation", *J. Chem. Phys.*, **107**, 524 (1997).

2. R. E. Larsen, G. Goodyear, and R. M. Stratt, "Liquid Theory for the Instantaneous Normal Modes of a Liquid II. Solutions", *J. Chem. Phys.*, **104**, 2987 (1996).

1. G. Goodyear, R. E. Larsen, and R. M. Stratt, "Molecular Origin of Friction in Liquids", *Phys. Rev. Lett.***76**, 243 (1996).

PATENTS

S. W. Hammond, D. C. Olson, R. E. Larsen and Z. Owczarczyk, "Organic Semiconductor Photovoltaic Devices and Compositions with Acceptor-Donor-Acceptor Type Polymer Electron Donors", Application No. PCT/US17/36714 (patent pending).

SELECTED CONFERENCE PROCEEDINGS

B. W. Larson, A. F. Ferguson, B. T. Tremolet de Villers, R. E. Larsen, "A Device-Independent Screening Technique for Rapidly Identifying Next Generation OPV Materials", *Proceedings of the 2017 PVSC-44*.

C. Zhang, F. Chen, M. H. Gray, R. Tirawat, R. E. Larsen,"The Effects of UV Aging on the Cracking of Titanium Oxide Layer on Poly (Ethylene Terephthalate) Substrate", *15th Biennial ASCE Conference on Engineering, Science, Construction, and Operations in Challenging Environments*, Earth and Space 2016.

S. Hammond, W. Braunecker, A. Garcia, R. E. Larsen, Z. Owczarczyk, D. Olson, and D. Ginley, "Oligomeric dithienopyrrole-thienopyrroledione (DTP-TPD) donor-acceptor copolymer for organic photovoltaics," *Record of the IEEE Photovoltaic Specialists Conference 2011*, 000712-000715.

S. R. Hammond, A. Garcia, A. Nardes, E. Knoll, M. Kose, R. E. Larsen, N. Kopidakis, Z. Owczarczyk, D. C. Olson, D. S. Ginley, "Triphenylamine-based star-shaped absorbers with tunable energy levels for organic photovoltaics", *Record of the IEEE Photovoltaic Specialists Conference 2010*, 001607-001610.

A. Rex and R. E. Larsen, "Entropy and Information for an Automated Maxwell's Demon," *PhysComp92*, Proceedings of the Workshop on Physics and Computation : October 2-4, 1992, pp. 93-101, (IEEE Press, 1993). Reprinted in *Maxwell's Demon 2: Entropy, Classical and Quantum Information, Computing*, A. F. Rex and H. S. Leff, eds. (Institute of Physics, New York, 2003).