

Neal R. Armstrong

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Director Emeritus, Institute for Energy Solutions (IES) <https://energy.arizona.edu/>

FIELDS OF SPECIALIZATION:

Interface Science of Materials for Energy Conversion, Light Emission and Sensing; Surface Photoemission Spectroscopies (UPS, XPS), Scanning Probe Microscopies, Electrochemistry, New Approaches to Development and Characterization of Energy Conversion Materials

ACADEMIC AND PROFESSIONAL APPOINTMENTS

- 2013 -2023 Regents Professor Chemistry/Biochemistry/Optical Sciences – University of Arizona – August 2013 –Sept. 2021 – Emeritus status (2021 – present)
<https://www.cbc.arizona.edu/faculty/neal-r-armstrong>
- 2023 - Affiliate Professor, Department of Chemistry, University of Washington
- 2015-2021 Director Arizona Institute for Energy Solutions (<https://energy.arizona.edu>)
- 2014-2020 Associate Vice President for Research – University of Arizona
- 2009- 2014 Director for the Department of Energy, Office of Science, Energy Frontier Center for Interface Science: Solar Electric Materials (CISSEM)
- 2002-07 Associate Director for the NSF Science and Technology Center Materials and Devices for Information Technology Research (MDITR)
- 1994 - 2000 Pacific Northwest Laboratories Affiliate Staff Scientist
- 1994 - Professor Optical Sciences, University of Arizona
- 1997-1999 Director, General Chemistry Laboratories, Department of Chemistry, Univ. Arizona
- 1989-1994 Head, Department of Chemistry, University of Arizona
- 1987- Professor, Department of Chemistry, University of Arizona
- 1982-87 Associate Professor, University of Arizona
- 1978-82 Assistant Professor, University of Arizona
- 1975-78 Assistant Professor, Michigan State University

EDUCATION

- 1970 B.S., Chemistry, University of New Mexico
- 1971-74 Associated Western Universities/Atomic Energy Commission Graduate Fellow at Sandia Laboratories, Albuquerque, New Mexico, in the Division of Solid State Physics Research
- 1974 Ph.D., Analytical Chemistry, University of New Mexico (Nick Vanderborgh/Rod Quinn)
- 1974-75 Ohio State University Postdoctoral Fellow (Ted Kuwana)

HONORS AND AWARDS

- 2013 Regents Professor in Chemistry/Biochemistry/Optical Sciences
- 2011 University of Arizona at the Leading-Edge Award – Innovation Day 2011
- 2011 Elizabeth and Keith Hege Galileo Circle Fellow – College of Science, University of Arizona
- 2002 Alexander von Humboldt Senior Research Prize – Institut für Angewandte Photophysik der Technischen Universität Dresden (IAPP)/Max Planck Institute für Polymerforschung – Mainz (MPIP)
- 2000 National Science Foundation - Special Award for Creativity, Chemistry
- 1996 Career Teaching Award, College of Science, University of Arizona
- 1996 National Science Foundation - Chemistry Special Award for Creativity
- 1992 Alexander von Humboldt Fellowship - Max Planck Institut für Polymerforschung
- 1985 Alexander von Humboldt Fellowship - Institut für Physicalische Chemie, Universität München

SCHOLARSHIP – RESEARCH INTERESTS

Over the last four decades my research activities have been primarily focused on enhancing our understanding of interfaces in materials and device platforms that are emerging (or have now emerged) as new technologies for solar energy conversion (solar cells), light emission (organic light emitting diodes), and chemical sensing platforms. We have played key roles in the development of new measurement science approaches to understanding the interfaces formed between these materials and metal, metal oxide and semiconductor electrical contacts, with primary emphasis on surface photoemission spectroscopies, electrochemistry and structural probes including X-ray diffraction, scanning probe microscopies and electron microscopies. As shown below the products of this scholarship have been 310+ peer-reviewed manuscripts and multiple patents, and the training of 49 Ph.D., ca. 25 M.S. and more than 100 undergraduate students, postdocs and visiting scientists. None of this would have been possible without significant collaborations and leadership from a group of like-minded scholars and educators from the University of Arizona, and scholars from research institutes around the world, including their students, postdocs and research scientists. Our program has been most impactful in the context of those collaborations. As can be seen below we have recently expanded or reinstated those interactions in a sustainable manner, also establishing new research activities in both the U.S. and Europe. Products of that scholarship are detailed below in the sections containing publications, patents, current and pending support, etc.

CONSULTING ACTIVITIES (since ca. 1980)

My consulting and scientific oversight and review activities, primarily in the areas of materials and interface characterization of optoelectronic, energy conversion and energy storage materials, have included both private companies and government laboratories, including: Burr-Brown, Sierracin-Sylmar, Motorola, Xerox, Kodak, IBM, 3M, Pacific Northwest Laboratories (PNNL), National Renewable Energy Laboratories (NREL), Brookhaven National Laboratories (BNL), Helmholtz-Zentrum Berlin.

Current and Pending Support and Recent Tech Transfer Activities

Current:

- Title: Understanding and Enhancing Stability of Perovskite/Contact Interfaces Across Length Scales
Summary: *This effort focuses on: 1) removal of surface defects at contact/perovskite active layer (PAL) interfaces using robust interface modification schemes; and 2) elucidation of complex degradation chemistries of rapidly evolving, high performing mixed cation halide perovskite active layers in PV platforms. – Ratcliff is lead/Armstrong participates either remotely or in person*
Source: Office of Naval Research
Period of Performance: 5/1/2018 – 5/17/2024
Total Award Amount: \$861,000
- Title: EMPOWER STEM: Electronic Materials to Power a Naval STEM Workforce
Summary: *This proposed effort is focused on establishing a unique training program at UA directed initially toward graduate students, and then at undergraduates to enable them to pursue career paths that lead to Department of Navy research laboratories, with active mentoring from DoN research scientists, partnering with UA faculty. – Ratcliff, Printz, Ogden are the lead PIs, Armstrong plays mostly a consulting off-site/in-person role at this point.*
Source: Office of Naval Research
Contract/Grant #: N/A
Annual Direct Costs: Year 1: \$249,608
Period of Performance: 02/01/21-01/31/24
Total Award Amount: \$748,824

- Title: “Advance Perovskite Solar Cell Development and Stability Using In-Line Electrochemical Methodologies”

Summary: *Overall Objectives: Develop and demonstrate a disposable, non-destructive electrochemical sensor prototype for: i) characterization of reactive defects in metal halide perovskite solar cell layers during in-line manufacturing (i.e., roll-to-roll) and ii) assessing quality, stability, and durability of device layers under stressors (i.e., humidity, light, and temperature).*

Source of Support: US DOE

Project/Proposal Support Start Date (if available): 10/1/2022

Project/Proposal Support End Date (if available): 09/30/2023

Total Award Amount (including Indirect Costs): \$300,000

Person-months per year committed 2023 0.18
- Title: **Center for Soft Photoelectrochemical Systems (SPECS)**

Summary: *This DOE Energy Frontier Research Center (EFRC) proposed effort is focused on the basic science underpinning the development of new materials, and their interfaces with electrolytes, for electrochemical and photoelectrochemical energy conversion and storage. Ratcliff (UA) Director and lead-PI, with Miller (NREL), Stinglein (Georgia Tech), Lian (Emory), Marder (CU).... et al. (Armstrong = Senior Advisor (UA)).*

Source: Department of Energy, EFRC

Award Amount: \$11M – August 2022-27.

Recent patent disclosures and patent assignments:

1. “Curriculum materials for the education of graduate level measurement science,” with Farrell, Heien, Saavedra, Armstrong, Oudry – Univ. of Arizona (UA19-115) – disclosure filed.
2. Organic Photovoltaic Devices Comprising Solution-Processed Substituted Metal Phthalocyanine and Exhibiting Near-IR Photo-Sensitivity, Dominic V. McGrath, Mayank Mayukh, Diogenes Placencia, Neal R. Armstrong US 9,505,770 B2
3. Conjugated Side-Strapped Phthalocyanines and Methods for Producing and Using the Same - US 9.425,413 B2
4. "Solar Window With Spectral And Photovoltaic Properties For Agricultural And Biofuel Applications," Lacombe, Peyghambarian, Ogden, Armstrong – UA16-085 - filed
5. “Compositions and Methods for Reducing Defects in Perovskite-Oxide Interface, Shallcross, Saavedra, Armstrong - UAZ -005700PV – filed
6. “Engineered Sorbents and Process for Selective Removal of Perfluorinated Organics Species from Water,” Karanikola et al. filed
7. “Device and Methods for Characterization of Semiconductor Films,” De Keersmaecker, et al. UAZ-008600PV – filed March 2022
8. “Defect Quantification in Metal Halide Perovskites – Projecting Photoluminescence and Photovoltaic Performance,” U.S. Provisional Patent Application No. 63/584,557, UA23-278 – filed Sept. 22, 2023

PAST STUDENTS

MS/Ph.D. (Ph.D. in bold; ** = joint students)

Mr. Vance Rogers Shepard, Duracell International Inc.
Mr. Curt Sayers, Semilab Inc.
Associate Prof. Clovis Linkous, Youngstown State University
Dr. Tom Mezza, Univ. Oil Prod., LLC
Dr. Robert Cieslinski, The Dow Chemical Company
Dr. Gary Deborski, Impact Analytical
Dr. David Hawn, The Dow Chemical Company
Dan Deibel, Adjunct Prof., Rochester Institute of Technology
Ken Chan – deceased (Cal St. Fresno Univ.)
Mr. Paul Lee (University of Arizona)
Dr. Ken Nebesny (University of Arizona)
Dr. Kevin Zavadil, SNL Sandia National Laboratories
Mr. Brad Thacker, LexisNexis
Dr. Tom Klofta, Proctor & Gamble Co.
Dr. Brian Maschhoff, Exelearn Systems, LLC
Dr. Peter Rieke, Pacific Northwest Laboratories
Dr. Michael Burrell, Bechtel Marine Propulsion Corp.
Mr. Tabitha Sims, Spectral Instruments, Inc
Dr. Joel Pankow, National Renewable Energy Laboratories
Dr. James Danziger, Proctor and Gamble Co.
Dr. Greg Collins, U.S. Naval Research Laboratory
Dr. Cory Hammond, Lexmark International, Inc.
Associate Prof. Elizabeth Atkinson, Linfield College **
Dr. Thomas Schuerlein, Evans Analytical Group Inc.
Dr. Lin Yang, Golden Sigma (Investment Management) **
Dr. Michelle Anderson, U.S. Naval Research Laboratory
Dr. Andrew Back, Physical Electronics Inc.
Dr. Paul Smolenyak, Yavapai College
Dr. Darren Dunphy, Sandia National Laboratories **
Dr. Jeff Anderson, Proctor and Gamble Co.
Dr. Peter Skrdla, Merck & Co., Inc. **
Dr. Rebecca (Peterson) Zangmeister, NIST
Dr. John Bradshaw, Artel Inc. **
Dr. Michael Hofmann, Technische Universität Dresden (Germany)
Dr. Carrie Donley, The University of North Carolina at Chapel Hill
Dr. Britt A. Minch, The Lubrizol Corp. **
Dr. Ware Flora, ConAgra Foods, Inc.
Dr. Wei Xia, China Business Executives Academy (China)
Dr. Beatrice Muriithi, Waters Corp.
Dr. Chet Carter, Micron Technologies

Dr. Chenhao Ge, DuPont Apollo Limited (China) **
Dr. Saneeha Marrikar, Huntsman Corp.
Dr. Michael Brumbach, Sandia National Laboratories
Dr. Sergio Paniagua-Barrantes, Intel Co.
Dr. Brooke Beam (University of Arizona) **
Prof. Dana M. Alloway, Concord University
Dr. Niranjani Kumaran, Samsung Austin Semiconductor
Dr. Clayton Shallcross (General Atomics)
Dr. P. Alexander Veneman, University of Texas at Austin
Dr. Adam Simmonds (University of Arizona)
Dr. Amy Graham (University of Arizona)
Dr. Diogenes Placencia, U.S. Naval Research Laboratory
Dr. Mariola Macech, Intel Co.
Dr. Judith Jenkins (Eastern Kentucky Univ.)
Dr. Brian Zacher, (University of Arizona)
Dr. Jeremy Gantz, Nike, Portland, OR
Dr. Gordon McDonald (NIST, Boulder, CO)
Dr. Kai-Lin Ou (Lamb Research, Portland, OR)
Dr. Michael Liao (Evans Associates, CA)
Dr. Mario Malfavon, Univ. Calif. San Diego
Ms. Xin Wu
Ms. Kara Saunders
Dr. James Stanfill, Nanoscience, Phoenix, AZ

Undergraduates

Kathleen Gibson (University Physicians)
Jim White (IBM), Roy Kaller (Gain Technologies)
Tom Patterson (pediatrician, Idaho), Deborah Kaller (Intel), John Fordemwalt (Hewlett-Packard)
Deborah Diehl, Michelle Douskey
Scott Waite (Proctor and Gamble), Cameron Oden, Shawn Kraut, Carole Mars (consultant)
Ron Buchanon (Motorola), Aaron Belsher (Micron)
Brian Nablo (NIST), Christina Hood (Penn State Univ.), Cathie Williamson, Jacob Woodruff
Matt Lawler, Ryan Hernandez (U.S. Navy)
Natalie Thompson, Cindy Taylor, Stephanie Tolbert, Kim Noble, Efram Zacusa, Avery Lindemann,
Brenda Molina, Brittany Lynn
Dan Huebner, Derek Manglesdorf, David Manglesdorf, Sonja Avetian McMenamin, Leo Hamerlynk

Postdocs/Visiting Faculty

Dr. William Butner, National Renewable Energy Laboratories (NREL)
Dr. Rosella Brina, consultant
Prof. Lai-Kwan Chau, National Chung-Cheng University (Taiwan)
Dr. Craig England, (Digital Electronics Corp.)

Prof. Claude Arbour, l'Université du Québec à Trois-Rivières (Canada)
Prof. Jean-Pol Dodelet, l'Université du Québec/INRS (Canada)
Dr. Valorie Valencia, Stellar Research Enterprises, Inc.
Dr. Albert Schmidt, Baumer Optronic GmbH
Prof. James Mills, Fort Lewis College
Prof. Hisao Yanagi, Kobe University (Japan)
Prof. Dr. Derek Schlettwein, Universität Giessen (Germany)
Prof. Rudiger Schlaf, University of South Florida
Prof. Marcus Lawrence, Concordia University (Canada)

Prof. Dr. Torsten Fritz, Universität Jena (Germany)
Dr. Liying Wang, BASF SE
Dr. Thomas Schulmeyer, SPECS Surface Nano Analysis, Inc.
Prof. Dana M. Alloway, Concord University
Prof. Erin Ratcliff (University of Arizona – Chemical Engineering)
Prof. Andrea Munro, Pacific Lutheran University
Prof. Weining Wang, Seton Hall University
Dr. Olga Griffith (Univ. Michigan)
Dr. Xerxes Steirer (Colorado School of Mines)
Dr. Clayton Shallcross (General Atomics)

PUBLICATIONS <https://orcid.org/0000-0003-1456-9612?lang=en>

312. “Reducing delamination of an electron-transporting polymer from a metal oxide for electrochemical application,” Aiswarya Abhisek, Mohapatra, Waleed Kuar Yual, Yadong, Zhang, Jonathan Thurston, Declan McCarthy, Casey M. Davis, Anton Aleksandrovich Samoylov, Adam D. Printz, Annie Greenaway, Michael F. Toney, Erin L. Ratcliff, Neal R. Armstrong, Stephen Barlow, Seth R Marder, Chem. Comm. in press - <https://doi.org/10.1039/D3CC05391A>
311. “Spectroelectrochemical Characterization of Energetics in Type I vs. Quasi-Type II Heterojunctions in CdSe@CdS Nanorod Films,” Dhruba Pattadar, Chisom Olikagu, Kyle J. Carothers, Jeffrey Pyun, S. Scott Saavedra, Neal R. Armstrong, Chemistry of Materials, in press - <https://doi.org/10.1021/acs.chemmater.3c02315>
310. “Defect Quantification in Metal Halide Perovskites Anticipates Photoluminescence and Photovoltaic Performance,” Michel De Keersmaecker, Juan Tirado, Neal R. Armstrong, and Erin L. Ratcliff, ACS Energy Letters, **2024**, 9, XXX, 243–252 - <https://doi.org/10.1021/acsenergylett.3c02157>
309. “Printing Our Energy Future: Soft Materials for Photoelectrochemical Fuel Production,” Erin L. Ratcliff, Zhiting Chen, Casey M. Davis, Eui Hyun Suh, Michael F. Toney, Neal R. Armstrong, Obadiah G. Reid, Ann L. Greenaway, ACS Energy Letters, November 2023 <https://doi.org/10.1021/acsenergylett.3c01782> .
308. “How low can you go? - Defect quantification at the 10^{15} cm⁻³ level in mixed-cation perovskites using differential pulse voltammetry,” Michel De Keersmaecker, Neal R. Armstrong, Erin L. Ratcliff, ACS Energy Lett., **2022**, 7, 4017-4027307; <https://doi.org/10.1021/acsenergylett.2c02033>
307. “Waveguide-Based Spectroelectrochemical Characterization of Band Edge Energies in Submonolayers of CdSe Quantum Dots Tethered to Indium-Tin Oxide Electrodes,” Weijun Sun, Chisom Olikagu, Kyle J. Carothers, Dhruba Pattadar, Jeffrey Pyun, S. Scott Saavedra, Neal R. Armstrong, Journal of Physical Chemistry C, **2022**, 126, 48, 20183–20195 <https://doi.org/10.1021/acs.jpcc.2c05692>
306. “Rationalizing Energy Level Alignment by Characterizing Lewis Acid/Base and Ionic Interactions at Printable Semiconductor/Ionic Liquid Interfaces,” Linze Du Hill, Michel De Keersmaecker, Adam E. Colbert, Joshua W. Hill, Diogenes Placencia, Janice E. Boercker, Neal R. Armstrong, and Erin L. Ratcliff, Materials Horizons, **2022**, 9, 471-481 DOI: 10.1039/D1MH01306H).
305. “Near-Surface Composition, Structure and Energetics of TiO₂ Thin Films: Characterization of Stress-Induced Defect States in Oxides Prepared via Chemical Vapor Deposition versus Solution Deposition from Sol-Gel Precursors,” R. Clayton Shallcross and Neal R. Armstrong, invited paper - J. Phys. Chem. C 2021, 125, 43, 24011–24024 -- DOI:10.1021/acs.jpcc.1c05477).

304. “Defect quantification in metal halide perovskites: The solid-state electrochemical alternative,” Michel De Keersmaecker, Neal R. Armstrong, and Erin L. Ratcliff, *Energy and Environmental Science*, **2021**, 14, 4840-4846 -- <https://doi.org/10.1039/D1EE01525G>
303. “Influence of Processing Environment on Surface Composition and Electronic Structure of Size-Quantized CdSe Quantum Dots,” R. Clayton Shallcross, Amy L. Graham, Metin Karayilan, Nicholas G. Pavlopoulos, Jordan Meise, Jeffrey Pyun and Neal R. Armstrong, *Journal of Physical Chemistry C* **124**, (2020) 21305-21308 - DOI: 10.1021/acs.jpcc.0c05622
302. “Reducing Surface Recombination Velocity of Methylammonium-Free Mixed-Cation Mixed-Halide Perovskites via Surface Passivation,” Sarthak Jariwala, Sven Burke, Sean Dunfield, Clayton Shallcross, Margherita Taddei, Jian Wang, Giles E. Eperon, Neal R. Armstrong, Joseph J. Berry, David S. Ginger, *Chemistry of Materials*, **2021**, 33, 13, 5035–5044 -- doi.org/10.1021/acs.chemmater.1c00848
301. “Overcoming redox reactions at perovskite/nickel oxide interfaces to boost voltages in perovskite solar cells,” Caleb C. Boyd, R. Clayton Shallcross, Taylor Moot, Ross Kerner, Luca Bertoluzzi, Arthur Onno, Shalinee Kavadiya, Cullen Chosy, Eli J Wolf, Jérémie Werner, James A Raiford, Camila de Paula, Axel F Palmstrom, Zhengshan J Yu, Joseph J Berry, Stacey F Bent, Zachary C Holman, Joseph M Luther, Erin L. Ratcliff, Neal R Armstrong, Michael McGehee, *Joule*, **4** (2020), 1-4 DOI:10.1016/j.joule.2020.06.004
300. “Zinc Phthalocyanine-Phosphonic Acid Monolayers on ITO: Influence of Molecular Orientation, Aggregation, and Tunneling Distance on Charge Transfer Kinetics, Luis E. Oquendo, Ramanan Ehamparam, Neal R. Armstrong, S. Scott Saavedra, Dominic V. McGrath, *J. Phys. Chem. C*. **123**, 6970-6980 (2019) DOI:10.1021/acs.jpcc.8b10301
299. “Impact of TiO₂ surface defects on the interfacial composition and energetics of evaporated perovskite active layers” R. Clayton Shallcross, Selina Olthof, Klaus Meerholz, Neal R. Armstrong, *ACS Applied Materials and Interfaces* **2019**, 11, 35, 32500–32508; DOI: 10.1021/acsami.9b09935
298. “Challenges and Opportunities at the Nexus of Energy, Water and Food,” N.R. Armstrong, R. Clayton Shallcross, Kimberly Ogden, Shane Snyder, Andrea Achilli, Erin L. Armstrong, *MRS Energy and Sustainability* (www.mrs.org/energy-sustainability-journal) **5**, (2018) DOI:10.1557/mre.2018.2
297. “Critical interface states controlling rectification of ultrathin NiO-ZnO p-n heterojunctions,” K. Xerxes Steirer, Kai Lin Ou, Paul Lee, Neal R. Armstrong, and Erin L. Ratcliff, *ACS Applied Materials and Interfaces*, **9**, 31111–31118 (2017) DOI: 10.1021/acsami.7b08899
296. “Axially Bound Ruthenium Phthalocyanine Monolayers on Indium Tin Oxide: Structure, Energetics and Charge Transfer Properties,” Ramanan Ehamparam, Luis E. Oquendo, Michael W. Liao, Ambjorn K. Brynne, Kai-Lin Ou, Neal R. Armstrong, Dominic V. McGrath, and S. Scott Saavedra, *ACS Applied Materials & Interfaces*, **9**, 29213-29223 (2017) DOI: 10.1021/acsami.7b07394
295. “Determining Band-edge Energies and Morphology-Dependent Stability of Formamidinium Lead Perovskite Films Using Spectroelectrochemistry and Photoelectron Spectroscopy,” R. Clayton Shallcross, Yilong Zheng, S. Scott Saavedra, N.R. Armstrong, *J. Amer. Chem. Soc.* **139** 4866-4878 (2017) DOI: 10.1021/jacs.7b00516.
294. “Introduction: Electronic Materials,” Erin Ratcliff, R. Clayton Shallcross, N.R. Armstrong, *Chemical Reviews*, **116**, 12621-12622 (2016) DOI: 10.1021/acs.chemrev.6b00646
293. “Surface modification of indium-tin oxide with functionalized perylene diimides: Characterization of orientation, electron-transfer kinetics and electronic structure,” Yilong Zheng, Anthony J. Giordano, R. Clayton Shallcross, Sean R. Fleming, Stephen Barlow, Neal R. Armstrong, Seth R. Marder, S. Scott Saavedra, *J. Phys. Chem. C*. **120**, 20040–20048 (2016) DOI: 10.1021/acs.jpcc.6b06812
292. “Characterization of ZnO Interlayers for Organic Solar Cells: Correlation of Electrochemical Properties with Thin Film Morphology and Device Performance,” Kai-Lin Ou, Ramanan Ehamparam, Gordon MacDonald, Tobias Stubhan, Xin Wu, R. Clayton Shallcross, Robin Richards, Christoph J. Brabec, S. Scott Saavedra, and Neal R. Armstrong, *ACS Applied Materials & Interfaces*, **8**, 19787-19798 (2016) DOI: 10.1021/acsami.6b02792

291. “Phosphonic acids for interfacial engineering of transparent conductive oxides,” Sergio A. Paniagua, Anthony J. Giordano, O’Neil L. Smith, Stephen Barlow, Hong Li, Neal R. Armstrong, Jeanne E. Pemberton, Jean-Luc Brédas, David Ginger, and Seth R. Marder, *Chemical Reviews*, 116, 7117–7158, (2016) DOI: 10.1021/acs.chemrev.6b00061.
290. “Overcoming Electrode Induced Losses in Organic Solar Cells by Tailoring a Quasi-Ohmic Contact to Fullerenes via Solution-Processed Alkali Hydroxide Layers,” Hong Zhang, R. Clayton Shallcross, Ning Li, Tobias Stubhan, Yi Hou, Wei Chen, Tayebah Ameri, Mathieu Turbiez, Neal R. Armstrong, Christoph J. Brabec, *Advanced Energy Materials*, 6, 1502195, (2016), DOI: 10.1002/aenm.201502195
289. “Solution Processed Titanyl Phthalocyanines as Donors in Solar Cells: Photoresponse to 1000 nm,” Mayank Mayukh, Mariola R. Macech, Diogenes Placencia, Yu Cao, Neal R. Armstrong, and Dominic V. McGrath, *ACS Applied Materials and Interfaces*, 9, 8786-8800 (2015), DOI: 10.1021/acsami.5b05900.
288. “Investigation of ultra-thin titania films as hole-blocking contacts for organic photovoltaics,” Hyungchul Kim, Kai-Lin Ou, Xin Wu, Paul F. Ndione, Joseph Berry, Yannick Lambert, d Thierry Melin, Neal R. Armstrong and Samuel Graham, *J. Mater. Chem. A*, 3, 17332-17343, (2015), DOI: 10.1039/c5ta04687d
287. “Characterization of Band Edge Energetics and Rates of Charge Injection Processes in Heterostructured Nanorods: Photoemission Spectroscopy and Waveguide Spectroelectrochemistry of Au-Tipped CdSe Nanorod Monolayers,” Ramanan Ehamparam, Nicholas Pavlopoulos, Michael W. Liao, Lawrence J. Hill, Neal R. Armstrong, Jeffrey Pyun, S. Scott Saavedra, *ACS Nano*, 9, 8786–8800, (2015); DOI: 10.1021/acsnano.5b01720
286. “Influence of Molecular Orientation on Charge-Transfer Processes at Phthalocyanine/Metal-Oxide Interfaces and Relationship to Organic Photovoltaic Performance,” Hsiao-Chu Lin, Gordon A. MacDonald, Yanrong Shi, Nate W. Polaske, Dominic V. McGrath, Seth R. Marder, Neal R. Armstrong, Erin L. Ratcliff, S. Scott Saavedra, *J. Phys. Chem. C*, 119, 10304-10313 (2015) DOI: 10.1021/acs.jpcc.5b02971
285. “Quantifying the Extent of Contact Doping at the Interface between High Work Function Electrical Contacts and Poly(3-hexylthiophene) (P3HT), R. Clayton Shallcross, Tobias Stubhan, Erin L. Ratcliff, Antoine Kahn, Christoph J. Brabec, Neal R. Armstrong, *J. Phys. Chem. Lett.* 6, 1303-09 (2015) DOI: 10.1021/acs.jpcclett.5b00444
284. “Nickel oxide interlayer films from nickel formate-ethylenediamine precursor: Influence of annealing on thin film properties and photovoltaic device performance,” K. X. Steirer, R. E. Richards, A. K. Sigdel, A. Garcia, P. F. Ndione, S. Hammond, D. Baker, E. L. Ratcliff, C. Curtis, T. Furtak, D. S. Ginley, D. C. Olson, N. R. Armstrong, J. J. Berry, *J. Materials Chemistry A*, 3, 10949–10958, (2015), DOI: 10.1039/c5ta01379h.
283. “Pentafluorophenoxy Boron Subphthalocyanine (F₅BsubPc) as a Multifunctional Material for Organic Photovoltaics,” Graham E. Morse, Jeremy L. Gantz, K. Xerxes Steirer, Neal R. Armstrong, and Timothy P. Bender, *ACS Applied Mater. Int.*, 6, 1515-1524 (2014), DOI: 10.1021/am404179z
282. “Structure-Processing-Property Correlations in Solution-Processed, Small-Molecule, Organic Solar Cells,” Benjamin H. Wunsch, Mariacristina Rumi, Naga Rajesh Tummala, Chad Risko, Dun-Yen Kang, Xerxes Steirer, Jeremy Gantz, Marcel M. Said, Neal Armstrong, Jean-Luc Brédas, David Bucknall, and Seth Marder, *Journal of Materials Chemistry C*, 1, 5250 - 5260 (2013), DOI: 10.1039/C3TC30774C.
281. “Organic Solar Cells – At The Interface,” Brian Zacher, Jeremy L. Gantz, Robin E. Richards, Neal R. Armstrong, Invited Commentary for the *Journal of Physical Chemistry Letters*, 4, 1949–1952, (2013), DOI: 10.1021/jz4009932.
280. “Energy level alignment and morphology of Ag and Au nanoparticle recombination contacts in tandem planar heterojunction solar cells,” K. Xerxes Steirer, Gordon A. MacDonald, Selina Olthof, Jeremy Gantz, Erin L. Ratcliff, Antoine Kahn, Neal R. Armstrong, *J. Phys. Chem. C.*, Invited (Ron Naaman Festschrift), 2013 DOI:10.1021/jp402672j
279. “Titanium Dioxide Electron-Selective Interlayers Created by Chemical Vapor Deposition for Inverted Configuration Organic Solar Cells,” Kai-Lin Ou, Delvin Tadytin, K. Xerxes Steirer,

Diogenes Placencia, Mike Nguyen, Paul Lee, and Neal R. Armstrong, *J. Mater. Chem. A*, **1**, 6794–6803 (2013), DOI: 10.1039/C3TA10894E.

278. “Influence of Electrode Surface Composition and Energetics on Small-Molecule Organic Solar Cell Performance: Polar Versus Non-Polar Donors on ITO Contacts,” Jeremy Gantz, Diogenes Placencia, Anthony Giordano, Seth R. Marder, Neal R. Armstrong, *J. Phys. Chem. C.*, 117 1205–1216 (2013). DOI: 10.1021/jp307546v.
276. “Electrical Property Heterogeneity at Transparent Conductive Oxide/Organic Semiconductor Interfaces: Mapping Contact Ohmicity Using Conducting-Tip Atomic Force Microscopy,” Gordon MacDonald, P. Alex Veneman, Diogenes Placencia, Neal R. Armstrong, *ACS Nano* **6**, 9623–9636, (2012). DOI: 10.1021/nn303043y.
275. "Built-in Potential in Conjugated Polymer Diodes with Changing Anode Work Function: Interfacial States and Deviation from the Schottky-Mott Limit," Bradley MacLeod; Noah Horwitz; Erin Ratcliff; Judith Jenkins; Neal R. Armstrong; Anthony Giordano; Peter Hotchkiss; Seth Marder; Charles Campbell; David Ginger, *J. Phys. Chem. Lett.*, **3**, 1202–1207, (2012) DOI: 10.1021/jz300283h
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SELECTED LEADERSHIP/SERVICE ACTIVITIES

A) Associate Vice President for Research University of Arizona: 2015/2020: During this period I assisted in i) the development of new research initiatives, scholarly activities and faculty hiring; ii) provided leadership and oversight of UA Core Facilities, developed new University Cores and upgraded existing cores and, iii) accelerated activities to enhance the pace and breadth of acquisition of new shared instrumentation through extramural funding.

1) **Research Development/Strategic Planning:** From 2014-20 the SVPR and AVPRs in RDI focused on areas of UA strength, or aspirational strength, in: Optics and Photonics (and more recently Quantum Information Science), Space Sciences, Imaging, Water/Energy/Arid Environments, Defense and Security, Informatics, and Translational Biosciences (accompanied by a parallel SP process in our Health Sciences colleges). Products of these planning activities were key in guiding research investment at UA over that period, including new faculty hiring (including “cluster hires”), and new core facilities, instrumentation and research infrastructure. We systematically worked with groups of faculty and research staff to develop strategies for growth of research in new areas and took the first steps to establish a “culture of research development” at UA in general.

My most rewarding activities involved the development of new research capacity in materials for quantum information science (QIS), and in energy conversion and water re-use/purification. We interfaced with our Washington D.C. consulting firm, and Federal Relations staff, to make sure we were apprised of changing opportunities and challenges to the funding landscape. Most importantly we focused on making sure that our young and mid-career faculty were getting the kind of support from RDI that they need to be successful and grow their programs, first of all in their core disciplines and secondly in these emerging cross-disciplinary activities.

2) **Core Facilities:** From 2014-20 I had oversight of a significant investment in new and established core research facilities, for physical, biological and health science activities, based on principles of uniqueness, enabling new research directions and hires, full accessibility to all researchers, coupled with sustainable and robust business practices. These efforts are tightly coupled with new faculty hiring and the implementation of new strategic research initiatives. New core facility capabilities included: i) Optical Microscopy, Electron Microscopy; ii) Mass Spectrometry for Proteomics/Lipidomics/Metabolomics and Small Molecule (drug discovery, new materials); iii) Molecular Structure (protein crystallography/high-field NMR), and Scanning Probe Microscopies (Keck Center for Nanoscale Imaging); iv) Clean Room/Micro- and Nano-fab and Functional Genomics; v) oversight of the implementation of the complex Translational Bio-Imaging Resource (TBIR) in our new Biosciences Research Laboratories (BSRL), opening early 2018.

B) Co-Director of the Institute for Energy Solutions (IES) – www.energy.arizona.edu -- In close collaboration with Kim Ogden we built research capacity in energy science/technology/policy at UA, transforming what had been the UA Renewable Energy Network (UAREN) into a more robust institute, with a significantly broader impact, and with an evolving emphasis on Energy/Water/Food Nexus issues, rather than just on energy. Our focus was to: i) intensify the networking of faculty expertise at UA to compete for more and larger sources of extramural funding, and to enhance impact to the citizens of Arizona and; ii) enhance the contact between the public and the faculty/staff and students of IES. In addition to the enhancement of research capacity and funding (ROI = ca. 5:1) our most notable outreach achievements are the **IES Energy Talks** (Stephanie Sikora/Will Holmgren/Cara Duncan) – “Scientists at SkyBar Talking Energy,” <https://energy.arizona.edu/events/304-ies-energy-talks> and the continued development of the **Arizona Student Energy Conference (AzSEC)**, which we started in 2010 as a partnership with Arizona State University, and expanded to include Northern Arizona University and more recently three universities within Mexico (Universidad Nacional Autónoma (UNAM), Universidad de Sonora, and Instituto Tecnológico y de Estudios Superiores de Monterrey -- <https://energy.arizona.edu/azsec-2019>

C) Director for the DOE Energy Frontier Center for Interface Science: Solar Electric Materials (CISSEM) – 2009-2014 (<http://science.energy.gov/bes/efrc/centers/cissem/>). Starting in 2008 I assembled a team of scholars in Chemistry, Optical Sciences, Physics, Materials Science and Electrical/Mechanical Engineering, at four universities and one national laboratory (Univ. Arizona, Georgia Tech, Princeton,

Washington, NREL) to form a Department of Energy -funded Energy Frontier Research Center (EFRC) – acting as the lead P.I. and Director. The Center was funded from 2009-2014 and I was Director and chief liaison between our center and DOE. Along with a Managing Director, Program Coordinator, and Business Office support, I managed a \$15M 5-year budget, and was responsible for setting the scientific direction of the center (14 P.I.s), ca. 65 total faculty, graduate students and postdocs/research scientists), the creation and articulation of our Mission and Strategic Plan, and assessment of our progress. I also managed our interactions with the public, and help coordinated the activities of the Energy Science Group (graduate and undergraduate students at UA interested in energy science, engineering, and renewable energy policy), in collaboration with the Renewable Energy Network (UA-REN).

Our **Strategic Plan** focused our research on four “Goal” areas: *i)* New theories to describe charge transfer between molecular semiconductors and electrical contact or interlayer materials; *ii)* New methodologies for the characterization of the atomic and molecular composition of interfaces, and new approaches for the nanoscale characterization of electrical and electrochemical properties of these interfaces; *iii)* New nanostructured hybrid materials that lead to the formation of chemically and physically robust interfaces; *iv)* New device platforms. CISSEM produced > 140 publications in high impact journals, and graduated more than 60 Ph.D. and M.S. graduate students, postdocs and visiting scientists. All are placed in high quality research positions, throughout the world.

D) Associate Director for the National Science Foundation – Science and Technology Center – Center for Materials and Devices for information Technology (CMDITR) – the Science and Technology Center for Materials and Devices for Information Technology Research began in 2002 with the University of Washington as the lead institution, and the University of Arizona, and the Georgia Institute of Technology as the secondary leads, with a host of other minority serving institutions as partners. I was the Associate Director for the University of Arizona effort for Years 2-5, and the Associate Director for Education for the first three years of this grant. This ca. \$32M effort (10 years – ca. 25 P.I.’s) produced a wide range of basic science results underpinning the development of new optical materials for telecommunications, broadly defined, and for the creation of new light emitting and energy conversion platforms, focusing on organic semiconductor and photonic materials. The last four years of this effort provided the springboard for funding of our EFRC, focusing on the development of new organic solar cell materials, and the interface science underpinning the optimization of their efficiencies and lifetimes. Details of our efforts can be found at <http://stc-mditr.org/>. This center had a significant educational/outreach component which I helped to direct in the first 5 years of the center (see below). Some of the products of that educational initiative are available at <http://stc-mditr.org/education/index.cfm>.

E) Department Head, Department of Chemistry, University of Arizona -- 1988-1994 -- I guided a Chemistry department with ca. 36 faculty members, ca. 200 graduate students and postdocs and ca. 50 undergraduate majors, ca. 24,000 student credit hours of undergraduate instruction, and ca. 200 support staff, through a tumultuous transition of departmental leadership, to help form a competitive, modern department. During this initial period of budget austerity for Arizona and UA specifically (a trend which has now continued for over 20 years), and with the help of excellent support staff (including an excellent Department Operations Manager), we still hired several key faculty and key research and teaching support staff and solidified the department’s operational procedures to include faculty in decision making and goal setting, while retiring a substantial debt left by previous administrations. We also developed our first Affirmative Action hiring plan and our first codified budget. Operating units were established with separate budget lines within the department, and Arizona Board of Regents-consistent performance assessment procedures, for both faculty and staff were fully implemented. And it should be mentioned that we retired a ca. 550K structural budget deficit which we inherited in 1988. This all seems like standard procedure now but was challenging to implement at the time.

Other significant University of Arizona leadership activities from previous years:

- ***University Committee on Ethics and Commitment*** (1997-2000, Chair of this committee 1999-2000). This was one of the most challenging service assignments that I have ever undertaken, and pre-dated a real, fully staffed Compliance Office. During this period this committee attempted to

act as mediator and grand jury to the Committee on Academic Freedom and Tenure, at a time when high profile cases of faculty/staff malfeasance were being adjudicated at UA.

- **Faculty Senate** (1998 - 2002)
- **College of Science Committee on Promotion and Tenure** (1998 – 2001; Head 2000/2001)
- **Intellectual Property Advisory Committee** (1990-2005) At the request of the Vice President for Research, I served on this committee for 15 years, acting in an advisory capacity and also helping to set research and intellectual property policy for UA, to establish a Conflict of Interest and Commitment Policy now in place for all of UA, and to anticipate problems arising as a result of changes in Federal rules and guidelines affecting the Office of Technology Transfer.
- **UA Research Policy Committee** (2007-09) – This was a committee convened in the transition between Vice-President’s for Research where advice and counsel was sought from research active faculty across campus.
- **Advance Program Advisory Committee and Leadership Group** (2007- 2013) -- One of my most visible and high impact roles during my tenure was the development of a seminar (with Professor LuAnn Gerken) on “**How to write a successful research proposal.**” We continue to run this presentation to a packed audience each time it is offered (ca. once per year).

PROFESSIONAL ACTIVITIES/SOCIETIES (only most recent)

- Editorial Advisory Boards -- Chemistry of Materials 1989-97, Langmuir 1985-89, Analytical Chemistry 2006-2009; Journal of Physical Chemistry 2013 – present; ACS Applied Electronic Materials 2018 – present
- Member of the Scientific Advisory Board for The Center for Hybrid Approaches in Solar Energy (CHASE), a DOE Energy Innovation Hub, UNC Chapel Hill, 2021-present
- Member of the External Advisory Board Nanotechnology Collaborative Infrastructure Southwest (NCI-SW) – 2018-present
- Director, Institute for Energy Solutions – July 1, 2018 – 2021 – Director Emeritus 2021 -
- 2018 Scientific and Technical Review of the Joint Center for Artificial Photosynthesis (JCAP) -- Cal Tech/LBNL/UC Berkeley – May 2018
- International Review Committee for “Energy” - Helmholtz-Zentrum Berlin für Materialien und Energie” (HZB) – Jan/Feb 2018
- Strategic Planning Committee for the Division of Materials Research, Optical and Photonic Materials (OPM) – National Science Foundation – Oct. 2017
- Strategic Planning Committee – Basic Research Needs (BRN) for Energy/Water – Department of Energy – Office of Science – Jan 2017
- Co-Chair Honors Dean Search Committee (UA) - 2017
- Chair, External Advisory Board for the UNC-Chapel Hill EFRC – “Center for Solar Fuels,” – August 2015 – 2019
- Advisory Board Member Institute for the Environment – 2017 - 2019
- Galileo Circle Fellows Advisory Council – College of Science UA – March 2019 - 20
- UA Committee on Innovation – part of the Strategic Planning process at Univ. Arizona – 2013/15
- UA RCM2 Committee – VPR/Indirect Cost Recovery – 2013/14
- Advisory Board Member - The Micro/Nano Fabrication Center, University of Arizona – 2013
- EMSL/Pacific Northwest Nat’l Labs – Advisory Board – 2002 – 2012
- Numerous Review Panels since 1980 for NSF, DOE, NIH
- Member: American Chemical Society; Materials Research Society