Sahar Sharifzadeh

Project Scientist, Theory of Nanostructured Materials
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Education

PhD Princeton University, Electrical Engineering, 2009
Supervisor: Emily A. Carter

MA Princeton University, Electrical Engineering, 2005

BS University of California, Berkeley, Electrical Engineering and Computer Science, 2003
Research Supervisor: Roger T. Howe

Research Experience

Project Scientist, Lawrence Berkeley National Laboratory, 5/2012 – present
Group of Jeffrey B. Neaton

- Lead role in research projects in the field of organic optoelectronics and excited-state theoretical method development
- Established new collaborations with experimentalists and theorists within the User Program of the Molecular Foundry
- Mentored graduate students and postdoctoral fellows
- Contributed to proposals and other research-related review documents

Postdoctoral Fellow, Lawrence Berkeley National Laboratory, 8/2009 – 5/2012
Supervisor: Jeffrey B. Neaton

- Explained and developed a model for exciton delocalization within organic solids, using many-body perturbation theory
- Provided a quantitative perspective on recent controversial interpretations of photoemission and inverse photoemission data
- Determined the relationship between interface electronic structure and organic photovoltaic device performance
- Explored the limits of current state-of-the-art first-principles methods for describing excited states in organics
- Developed additional functionality in the open-source *BerkeleyGW* many-body perturbation theory package (berkeleygw.org)

Graduate Research Assistant, Princeton University, 7/2005 – 8/2009
Supervisor: Emily A. Carter

- Developed and tested an all-electron embedded cluster simulation method to go beyond a density functional theory description of localized features in condensed matter
- Resolved an uncertainty regarding the failure of standard theoretical methods in describing CO adsorbed on transition metals
- Explained trends in the scanning tunneling spectroscopy lineshape of Kondo impurities

Graduate Research Assistant, Princeton University, 1/2004 – 7/2005
Supervisor Antoine Kahn

- Studied chemistry at metal-organic interfaces via photoemission spectroscopy

Undergraduate Research Assistant, UC Irvine, 6/2003 – 8/2003
Supervisor Richard Nelson

- Characterized and fabricated PDMS microsprings for applications to a Fabry-Perot optical filter

Undergraduate Research Assistant, UC Berkeley, 8/2001 – 5/2003
Supervisor: Roger T. Howe

- Characterized the hydrophilicity of PDMS-based thin films for application to a microelectro-mechanical system (MEMS) bio-reactor
- Designed a printed circuit board for large-scale production of MEMS bio-reactor

Mentoring Experience

Molecular Foundry, Lawrence Berkeley National Laboratory

- Mentor to graduate students Samia Hamed and Florian Altvater (UC Berkeley) in the Neaton group
- Co-advisor to undergraduate/post-graduate student Eric B. Isaacs (UC Berkeley) culminating in a *J. Phys. Chem. Lett.* publication
- Associate mentor to Amaresh Sahu (Princeton University) through the Science Undergraduate Laboratory Internship (SULI) program

Princeton University

- Mentor to Jason Kawasaki (Princeton University) for junior thesis project

Teaching Experience

Educational Tool Developer, nanoHub.org, 2009 – 2012

- BerkeleyGW simulation tool
- Organic photovoltaics educational tool

Resident Graduate Tutor, Whitman College, Princeton University, 2007 – 2008

- Informally advised and interacted with undergraduate students
- Led math/physics/electrical engineering discussion tables and tutoring sessions during Fall 2007

Assistant in Instruction, Princeton University, Fall 2005

- Introductory materials science course (MAE 324)
- Responsibilities included running a 1-hour discussion session every two weeks, generating and grading of problem sets, and grading exams

Physics Scholars Program Tutor, UC Berkeley, 2002 – 2003

- Introductory Physics for non-majors (Physics 8A/B)
- Responsible for running one 2-hour discussion session per week with one other tutor

Invited Presentations

- "Understanding the Spectroscopic Properties of Organic Semiconductors from First-Principles," *University of Arkansas, Dept. of Physics*, Fayetteville, AR, 10/16/2013
- "Tuning the Opto-Electronic Properties of Organic Semiconductors via Solid-State Morphology," *University of California, Santa Barbara, Materials Dept*., Santa Barbara, CA, 10/2/2013
- "First-Principles Design of Excited-State Properties in Organic Materials," *University of Minnesota, Dept. of Electrical and Computer Engineering*, Minneapolis, MN, 9/5/2013
- "First-Principles Design of Excited-State Properties in Organic Materials," *University of Illinois, Urbana-Champaign, Dept. of Materials Science and Engineering*, Urbana, IL, 1/24/2013

- "A First-Principles Approach to Understanding Excited State Properties of Organic Systems," *Molecular Foundry Seminar Series*, Berkeley, CA, 12/11/2012
- "Excited States in Organic Donor/Acceptor Assemblies," *Molecular Foundry User Executive Committee Monthly Meeting*, Berkeley, CA, 11/1/2012
- "First-Principles Studies of the Electronic Structure of Organic Semiconductors and Interfaces," *The Molecular Foundry & the National Center for Electron Microscopy Users' Meeting 2010*, Berkeley, CA, 10/1/2010

Selected Contributed Presentations

- **Speaker:** S. Sharifzadeh, P. Darancet, L. Kronik, and J.B. Neaton, "Understanding the Nature of Excitons in Organic Semiconductors from First Principles," *Organic Solar Cells: Theory and experiment, from Description to Prediction,* Santa Fe, NM, 5/8/2013
- **Poster Presentation:** S. Sharifzadeh, L. Kronik, and J.B. Neaton, "Excited States of Organic Donor/Acceptor Materials from First-Principles," *The 7th Edition of the International Workshop on Electronic Structure and Processes at Molecular-Based Interfaces (ESPMI VII)*, Rehovoth, Israel, 5/1/2013
- **Speaker:** S. Sharifzadeh, P. Darancet, L. Kronik, and J.B. Neaton, "Relating Crystal Structure and the Charge-Transfer Nature of Excitons in Pentacene from First Principles," *American Physical Society March Meeting*, Baltimore, MD, 3/19/2013
- **Speaker:** S. Sharifzadeh, L. Kronik, and J.B. Neaton, "Visualizing Excitons in Pentacene and Perfluoropentacene Donor-Acceptor Blends with Computational Spectroscopy," *2012 Materials Research Society Spring Meeting*, San Francisco, CA, 4/12/2012
- **Speaker:** S. Sharifzadeh, L. Kronik, and J.B. Neaton, "Relating Molecular-Scale Structure to Spectroscopy in Pentacene-Perfluoropentacene Donor-Acceptor Assemblies," *American Physical Society March Meeting*, Boston, MA, 3/2/2012
- **Poster Presentation:** S. Sharifzadeh, A. Biller, L. Kronik, and J.B. Neaton, "First-Principles Study of the Spectroscopy of the Organic Semiconductors Pentacene and PTCDA: Insight into Transport and Optical Excitations," *Organic Microelectronic and Optoelectronic Workshop VII*, San Francisco, CA, 7/18/2011
- **Speaker:** S. Sharifzadeh, A. Biller, L. Kronik, and J.B. Neaton, "Spectroscopy of Organic Semiconductors from First-Principles," *American Physical Society March Meeting*, Dallas, TX, 3/24/2011
- **Speaker:** S. Sharifzadeh, A. Biller, L. Kronik, and J.B. Neaton, "First-Principles Study of the Electronic Structure of Organic Crystals," *American Physical Society March Meeting*, Portland, OR, 3/18/2010
- **Poster Presentation:** S. Sharifzadeh, A. Biller, L. Kronik, and J.B. Neaton, "First-Principles Study of the Electronic Structure of Organic Crystals," *22nd Annual Workshop on Electronic Structure Methods*, Austin, TX, 6/9/2010
- **Speaker:** S. Sharifzadeh, P. Huang, and E.A. Carter, "Correlated Wavefunction Description of Kondo States on Metal Surfaces," *American Physical Society March meeting*, Pittsburgh, PA, 3/19/2009
- **Speaker:** S. Sharifzadeh, P. Huang, and E.A. Carter, "Embedded Configuration Interaction Description of Kondo States on Metal Surfaces," *American Chemical Society National Meeting*, Philadelphia, PA, 8/19/2008

Publications

PhD Dissertation

S. Sharifzadeh, "Embedded Correlated Wavefunction Description of Local Features within Condensed Matter," Princeton University, Princeton, NJ, 2009.

Submitted Manuscripts

- D.A. Egger, S. Weissman, S. Refaely-Abramson, S. Sharifzadeh, M. Dauth, R. Baer, S. Kummel, J.B. Neaton, E. Zojer, L. Kronik, "Outer-Valence Electron Spectra of Prototypical Organic Molecules from an Optimally-Tuned Range-Separated Hybrid Functional: A Quantitative Analysis, submitted to *J. Chemical Theory and Computation*"

Refereed Publications

- S. Refaely-Abramson, S. Sharifzadeh, M. Jain, R. Baer, J.B. Neaton, and L. Kronik, "Gap Renormalization of Molecular Crystals from Density Functional Theory," *Physical Review B* **88**, 081204(R) (2013).
- S. Sharifzadeh, P.T. Darancet, L. Kronik, and J.B. Neaton, "Low-Energy Charge-Transfer Excitons in Organic Solids from First-Principles: The Case of Pentacene," *J. Physical Chemistry Letters* **4**, 2197 (2013).
- S. Refaely-Abramson, S. Sharifzadeh, N. Govind, J. Autschbach, J.B. Neaton, R. Baer, and L. Kronik, "Quasiparticle Spectra from a Non-Empirical Optimally-Tuned Range-Separated Hybrid Density Functional," *Physical Review Letters* **109**, 226405 (2012).
- S. Sharifzadeh, I. Tamblyn, P. Doak, P. Darancet, and J.B. Neaton, "Quantitative Molecular Orbital Energies within a G_0W_0 Approximation," *European Physical Journal B* **85**, 323 (2012).
- S. Sharifzadeh, A. Biller, L. Kronik, and J.B. Neaton, "Quasiparticle and Optical Spectroscopy of Organic Semiconductors Pentacene and PTCDA from First Principles," *Physical Review B* **85**, 125307 (2012).
- D.K. Kanan, S. Sharifzadeh, and E.A. Carter, "Quantum Mechanical Modeling of Electronic Excitations in Metal Oxides: Magnesia as a Prototype," *Chemical Physics Letters* **519-520**, 18 (2012).
- E.B. Isaacs, S. Sharifzadeh, B. Ma, and J.B. Neaton, "Relating Trends in First-Principles Electronic Structure and Open-Circuit Voltage in Organic Photovoltaics," *J. Physical Chemistry Letters* **2**, 2531 (2011).
- S. Sharifzadeh, P. Huang, and E. A. Carter, "Origin of Tunneling Lineshape Trends for Kondo States of Co Adatoms on Coinage Metal Surfaces," *J. Physics: Condensed Matter* **21**, 355501 (2009).
- S. Sharifzadeh, P. Huang, and E.A. Carter, "All-Electron Embedded Correlated Wavefunction Theory for Condensed Matter Electronic Structure," *Chemical Physics Letters* **470**, 347 (2009).
- S. Sharifzadeh, P. Huang, and E.A. Carter, "Embedded Configuration Interaction Description of CO on Cu (111): Resolution of the Site Preference Conundrum," *J. Physical Chemistry C* **112**, 4649 (2008).
- M.M. Maharbiz, W.J. Holtz, S. Sharifzadeh, J.D. Keasling, and R.T. Howe, "A Microfabricated Electrochemical Oxygen Generator for High-Density Cell Culture Arrays," *J. of Microelectromechanical Systems* **12**, 590 (2003).
- M.M. Maharbiz, W.J. Holtz, S. Sharifzadeh, J.D. Keasling, and R.T. Howe, "A Microfabricated Electrochemical Oxygen Generator for High-Density Cell Culture Arrays," *Solid-State Sensors, Actuators, and Microsystems Workshop*, Hilton Head Island, SC, June 2-6, 259 (2002).

References

- **Emily A. Carter (PhD advisor)**
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  Princeton University
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