

# MICHELE KOTIUGA

## CONTACT INFORMATION

E-mail: [mkotiuga@physics.rutgers.edu](mailto:mkotiuga@physics.rutgers.edu)

## ADDRESS

Department of Physics and Astronomy  
Rutgers, The State University of New Jersey  
136 Frelinghuysen Road  
Piscataway, NJ 08854

Website: <http://www.physics.rutgers.edu/~mkotiuga/>

## RESEARCH INTERESTS

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- First-principles calculations of complex materials for energy and device applications
- Charge transport phenomena in real materials
- Many-electron and electrostatic contributions to electron structure at interfaces
- Controlling material properties through high concentration doping

## WORK EXPERIENCE

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April 2016 -

Postdoctorate Fellow: Supervisor Prof. Karin M. Rabe  
Rutgers, The State University of New Jersey

## EDUCATION

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### University of California, Berkeley

Ph.D. in Physics (December 2015), GPA: 4.0

Dissertation - "Charge Transport in Molecular Junctions: A Study of Level-Alignment, Thermoelectric Properties, and Environmental Effects"

Adviser: Jeffrey B. Neaton

M.A. in Physics (May 2010), GPA: 4.0

### Boston University

B.A. Magna Cum Laude in Physics with Distinction (May 2008)

Thesis - "Structural, Electronic, and Vibrational Properties of Carbon Nanotubes"

Adviser: Anna Swan

B.A. Magna Cum Laude in Mathematics (May 2008)

Cumulative GPA: 3.74

Physics: 3.98

Mathematics: 3.71

## SCHOLARSHIPS AND AWARDS

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- **2014 Molecular Foundry User Meeting Poster Award**
- **2013 Scholarship to Visit Universität Konstanz, Germany: funded by the DFG Excellence Initiative**

This award was given by the Deutsche Forschungsgemeinschaft to conduct research at Universität Konstanz for 4 months.

- **2011 Outstanding Graduate Student Instructor**

This award is given annually to a handful of graduate student instructors in each department. They are nominated by both supervising faculty and students.

- **2008 Class Prize in Physics, Boston University**

Given annually to the top graduating student in the department.

## PUBLICATIONS

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- **M. Kotiuga**, K. M. Rabe  
High-Concentration Electron doping of samarium nickelate from first principles.  
*Manuscript in prep.*
- **M. Kotiuga**, P. Darancet, J. B. Neaton  
Implicit modeling of changes to work function due to mixed monolayer passivation.  
*Manuscript in prep.*
- 8. Y. Sun\*, **M. Kotiuga\***, D. Lim, B. Narayanan, M. Cherukara, Z. Zhang, Y. Dong, R. Kou, C.-J. Sun, Q. Lu, I. Waluyo, A. Hunt, H. Tanaka, A. N. Hattori, S. Gamage, Y. Abate, V. G. Pol, H. Zhou, S. K. R. S. Sankaranarayanan, B. Yildiz, K. M. Rabe, S. Ramanathan  
Strongly correlated perovskite lithium ion shuttles  
*Proceedings of the National Academy of Sciences*, **2018**, 115, 9672 . (\* Equal Contributors)
- 7. Z. Zhang, D. Schwanz, B. Narayanan, **M. Kotiuga**, J. A. Dura, M. Cherukara, H. Zhou, J. W. Freeland, J. Li, R. Sutarto, F. He, C. Wu, J. Zhu, Y. Sun, K. Ramadoss, S.S. Nonnenmann, N. Yu, R. Comin, K. M. Rabe, S. K. R. S. Sankaranarayanan, S. Ramanathan  
Perovskite nickelates as electric-field sensors in salt water  
*Nature*, **2018**, 553, 68.
- 6. F. Zuo, P. Panda, **M. Kotiuga**, J. Li, M. Kang, C. Mazzoli, H. Zhou, A. Barbour, S. Wilkins, B. Narayanan, M. Cherukara, Z. Zhang, S. K. R. S. Sankaranarayanan, R. Comin, K. M. Rabe, K. Roy, and S. Ramanathan  
Habituation based synaptic plasticity and organismic learning in a quantum perovskite  
*Nature Communications*, **2017**, 8, 240.
- 5. **M. Kotiuga**, P. Darancet, C. R. Arroyo, L. Venkataraman, and J. B. Neaton  
Adsorption-induced solvent-based electrostatic gating of charge transport through molecular junctions.  
*Nano Letters*, **2015**, 15, 4498.
- 4. W. B. Chang\*, C.-K. Mai\*, **M. Kotiuga\***, J. B. Neaton, G. C. Bazan, and R. A. Segalman,  
Controlling the thermoelectric properties of thiophene-derived single-molecule junctions  
*Chemistry of Materials*, **2014**, 26, 7229. (\* Equal Contributors)
- 3. J. Lynch, **M. Kotiuga**, V. V. T. D.-Nguyen, W. L. Queen, J. D. Forster, R. A. Schlitz, C. B. Murray, J. B. Neaton, M. L. Chabynyc, and J. J. Urban.  
Ligand coupling symmetry correlates with thermopower enhancement in small-molecule/nanocrystal hybrid materials.  
*ACS Nano*, **2014**, 8, 10528.

2. B. Capozzi, Q. Chen, P. Darancet, **M. Kotiuga**, M. Buzzeo, J. B. Neaton, C. Nuckolls, and L. Venkataraman  
Tunable Charge Transport in Single-Molecule Junctions via Electrolytic Gating  
*Nano Letters*, **2014**, 14, 1400.
1. T. Kim, P. Darancet, J. R. Widawsky, **M. Kotiuga**, S. Y. Quek, J. B. Neaton, and L. Venkataraman  
Determination of energy level alignment and coupling strength in 4,4-bipyridine single-molecule junctions.  
*Nano Letters*, **2014**, 14, 794.

## TALKS AND SEMINARS

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### INVITED

**2017 Cavendish Laboratory, Cambridge University**, Cambridge, UK. Invited Seminar: “Electron doping of  $\text{SmNiO}_3$  from first principles.”

**2015 Chemistry Department, Princeton University**, Princeton, NJ. Car & Selloni Groups: Informal Seminar.

**2015 Physics and Applied Physics Departments, Columbia University**, New York, NY. Marianetti & Millis Groups: Informal Seminar.

**2015 Physics Department, Rutgers University**, New Brunswick, NJ. Rabe Group: Informal Seminar.

**2015 EPFL THEOS Seminar**, Lausanne, Switzerland. Invited Seminar: “Theory of solvent effects on charge transport in molecular junctions.”

**2014 Intel: Massachusetts Microprocessor Design Center** Hudson, MA. Invited Seminar: “Using *ab initio* calculations of electron transport to model and design molecular based devices.”

**2014 International Workshop on Controlled Charge and Heat Transport at the Molecular Scale**, Konstanz, Germany. Invited Talk: “Insight into charge transport in molecular junctions via *ab initio* theories of level alignment.”

### CONTRIBUTED

**2018 APS March Meeting**, Los Angeles, CA. “Modulation doping in  $\text{LaNiO}_3/\text{SrIrO}_3$  superlattices from first principles.” Session: Electronic Structure, Topological Effects and Magnetotransport in Complex Oxide

**2018 Fundamental Physics of Ferroelectrics**, Washington D.C., “A first-principles study of ferroelectricity in samarium nickelate with intercalated hydrogen.”

**2017 APS Mid-Atlantic Section Meeting** Newark, NJ. “Modulation doping in  $\text{LaNiO}_3/\text{SrIrO}_3$  superlattices from first principles.”

**2017 APS March Meeting**, New Orleans, LA. “Electron doping of  $\text{SmNiO}_3$  from first principles.” Session: Bulk Oxides

**2017 Fundamental Physics of Ferroelectrics**, Williamsburg, VA. “Electron doping and charge ordering of  $\text{SmNiO}_3$  from first principles.”

**2016 APS March Meeting**, Baltimore, MD. “Theory of work function tuning via mixed-monolayer on functional surfaces.” Session: Electron transport at nanoscale interfaces

**2015 APS March Meeting**, San Antonio, TX. “Self-energy-corrected electronic energy level alignment in molecular junctions and at interfaces with hybrid functionals.” Session: Energy and electron flow at interfaces in nanostructures.

**2014 APS March Meeting**, Denver, CO. “Length dependence of conductance and thermopower of hybrid alkyl-thiophene single molecule junctions.” Session: Electron, ion, and exciton transport in Nanostructures.

**2013 APS March Meeting**, Baltimore, MD. “Theory of solvent-mediated environmental effects on transport in molecular junctions.” Session: Mesoscopics - tunneling

**2012 APS March Meeting**, Boston, MA. “Theory of solvent-mediated environmental effects on molecular-scale Transport.” Session: Electron, ion, and exciton transport in Nanostructures - Junctions.

**2008 Conference for Undergraduate Women in Physics**, New Haven, CT. Structural, Electronic, and vibrational properties of carbon nanotubes.

## POSTER PRESENTATIONS

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**2018 Electronic Structure Workshop**, Pennsylvania, PA. “Modulation doping in  $\text{LaNiO}_3/\text{SrIrO}_3$  superlattices from first principles”.

**2017 Electronic Structure Workshop**, Princeton, NJ. “Electron doping of  $\text{SmNiO}_3$  from first principles”.

**2015 Batsheva de Rothschild Seminar on Molecular Electronics** Ma’ale Hachamisha, Israel. “Electronic energy level alignment in molecular junctions with standard DFT approaches, hybrid functionals, and model GW calculations”

**2014 International Workshop on Controlled Charge and Heat Transport at the Molecular Scale**, Konstanz, Germany. “Theory of Solvent Effects on Charge Transport in Molecular Junctions.”

**2014 Molecular Foundry User Meeting**, LBNL, Berkeley, CA. “Tuning level alignment and thermopower of thiophene based single-molecule junctions”. *Awarded a Poster Prize.*

**2013 CECAM Workshop: “Nanophononics”**, Bremen, Germany. “Tuning level alignment and thermopower of thiophene Based single-molecule junctions”

**2012 Molecular Foundry User Meeting**, LBNL, Berkeley, CA. “Understanding the role of environment on molecular-scale transport”

**2011 Molecular Foundry User Meeting**, LBNL, Berkeley, CA. “Understanding the role of environment on molecular-scale transport”

**2008 Conference for Undergraduate Women in Physics**, New Haven, CT. “Structural, electronic, and vibrational properties of carbon nanotubes.”

## COMMUNITY AND TEACHING EXPERIENCE

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Panelist

Women in STEM Professional &  
Career Panel Discussion  
Brookdale Community College

02/2017

Served as a panelist discussing my experiences as a physics student and in my career on a panel for STEM students at Brookdale Community College. The event, directed as women but open to all, was well attended with a lively discussion.

**Head Coordinator** Society of Women in the Physical Sciences 8/09–8/11  
UCB

Led the Society of Women in the Physical Sciences which includes students from the Physics, Astronomy, and Earth and Planetary Sciences Departments. Organized events and networking with female faculty and alumni and dinners for graduate students and postdocs, informational, community and mentoring events for undergraduates and community outreach programs.

**Graduate Student Instructor** Physics Department 8/08–5/11  
UCB

Physics 137A & 137B: Undergraduate Quantum Mechanics. Held discussions and graded homeworks and exams.

Physics 7A: Physics I for Scientists and Engineers. Held discussions and labs and graded exams.

Physics 8B: Introductory Physics II. Held discussions and labs and graded exams and was the head student instructor for the Fall 2010 semester.

## **PROFESSIONAL EXPERIENCE**

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**Undergraduate Co-op** Massachusetts Microprocessor Design Center 5/07–8/07  
Intel Corporation

Over the summer of 2007, I held a co-op position in the Massachusetts Microprocessor Design Center (MMDC) working on power analysis and modeling in microprocessors.