

# Sean M. Ryno: Curriculum Vitae

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## Business Address

2540 Research Park Drive  
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## Permanent Address

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## EDUCATION

### Georgia Institute of Technology

Ph. D., Chemistry

GPA: 3.42

Atlanta, GA

August 2015

Research Advisor: Professor Jean-Luc Brédas

Thesis: Molecular-Scale Understanding of Electronic Polarization in Organic Molecular Crystals

### University of North Georgia

B.S., Chemistry

GPA: 3.60 (Cum Laude)

Dahlonega, GA

May 2010

Research Advisors: Professor Dan Thompson and Professor Aimee Tomlinson

## ACADEMIC AWARDS

- William H. Emerson Fellowship (2010-2011)
- Summer Undergraduate Research Experience at Emory University Fellowship (2009)

## RESEARCH EXPERIENCE

### University of Kentucky

Post-Doctoral Scholar

Lexington, KY

11/2016-Present

Research Advisor: Professor Chad Risko

- Applying multiscale methodologies – including QM and MD – using GPUs to understand the structure-property relationships in a series of conjugated polymers.
- Parameterized forcefields to allow for the study of novel organic systems using molecular dynamics.
- Utilizing symmetry-adapted perturbation theory to develop an understanding of the interactions that drive molecular packing in small-molecule organic crystals.

### King Abdullah University of Science and Technology

Post-Doctoral Fellow / Student Researcher

Thuwal, KSA

08/2014-11/2016

Research Advisor: Professor Jean-Luc Brédas

- Applied a multiscale model of bulk polarization energy to model organic photovoltaic materials to capture the complex nature of the energetic landscape at the interface of these materials.

- Performed molecular dynamics simulations of model organic photovoltaic bilayer interfaces to obtain more realistic interface geometries as compared to previous systems composed of two slabs brought into close-contact.
- Extracted geometries from molecular dynamics snapshots to generate distributions of electronic couplings and charge transfer state energies to improve the understanding of interactions at organic-organic interfaces.
- Utilized symmetry-adapted perturbation theory to construct multidimensional potential energy surfaces of the oligoacenes (i.e., benzene through hexacene) to determine how non-bonded interactions change upon dimer transformation and as a function of acene length.

**Georgia Institute of Technology**

Atlanta, GA

Research Assistant

10/2010-07/2015

Research Advisor: Professor Jean-Luc Brédas

- Dissertation: Molecular-Scale Understanding of Electronic Polarization in Organic Molecular Crystals
- Developed multiscale model to determine the bulk polarization energies in organic molecular crystals.
- Explored polarization in oligoacenes. Multiscale model provides improved agreement compared with other theoretical techniques concerning experimentally observed polarization energies and the polarization asymmetry due to charges of different sign.
- Employed combined quantum-mechanical–molecular-mechanics methods to examine the nature of intermolecular interactions in organic crystals as a function of molecular structure and chemical substitution.

**University of North Georgia**

Dahlonega, GA

Research Assistant

01/2009-05/2010

Research Advisor: Professor Dan Thompson

- Synthesized a brominated aniline that changed color as a function of temperature, a phenomenon determined to be the result of an enol-keto tautomerization. Employed differential scanning calorimetry to determine the rate of the color change as a function of the number of heating cycles, the rate of back conversion, and the reproducibility of this conversion on the same sample.

Research Assistant

08/2009-05/2010

Research Advisor: Professor Aimée Tomlinson

- Carried out density functional theory calculations and investigated the electronic properties of a series of benzobisoxazoles.

**Emory University**

Atlanta, GA

Research Assistant

05/2009-07/2009

Research Advisor: Professor Simon Blakey

- Synthesized novel copper organometallic catalysts for C-H functionalization reactions and employed a series of analytical characterizations (NMR, Mass Spectrometry, HPLC, IR, UV-Vis) to investigate the structure-property relationships.

## TEACHING EXPERIENCE

### Georgia Institute of Technology

Teaching Assistant for Chemical Principles 1211K

Atlanta, GA

8/2010-5/2011

- Taught four sections of 1211K lab with tutoring sessions.

## PUBLICATIONS

1. **Ryno, Sean M.**; Lee, Stephen R.; Sears, John S.; Risko, Chad; and Brédas, Jean-Luc. "Electronic Polarization Effects upon Charge Injection in Oligoacene Molecular Crystals: Description via a Polarizable Force Field." *Journal of Physical Chemistry C*, **2013**, 117, 13853-13860.
2. **Ryno, Sean M.**; Risko, Chad; and Brédas, Jean-Luc. "Impact of Molecular Packing on Electronic Polarization in Organic Crystals: The Case of Pentacene vs TIPS-Pentacene." *Journal of the American Chemical Society*, **2014**, 136, 6421-6427.
3. **Ryno, Sean M.**; Risko, Chad; and Brédas, Jean-Luc. "Impact of Molecular Orientation and Packing Density on Electronic Polarization in the Bulk and at Surfaces of Organic Semiconductors." *ACS Applied Materials & Interfaces*, **2016**, 8, 14053-14062.
4. Haitao, Sun; **Ryno, Sean M.**; Zhong, Cheng; Ravva, Mahesh; Sun, Zhen-Rong; Körzförfer, Thomas; Brédas, Jean-Luc. "Ionization Energies, Electron Affinities, and Polarization Energies of Organic Molecular Crystals: Quantitative Estimations from a Polarizable Continuum Model (PCM)-Tuned Range-Separated Density Functional Approach." *Journal of Chemical Theory and Computation*, **2016**, 12, 2906-2916.
5. **Ryno, Sean M.**; Risko, Chad; and Brédas, Jean-Luc. "Non-Covalent Interactions and Impact of Charge Penetration Effects in Linear Oligoacene Dimers and Single Crystals." *Chemistry of Materials*, **2016**, 28, 3990-4000.
6. **Ryno, Sean M.**; Fu, Yao-Tsung; Risko, Chad; and Brédas, Jean-Luc. "Polarization Energies at Organic-Organic Interfaces: Impact on the Charge Separation Barrier at Donor-Acceptor Interfaces in Organic Solar Cells." *ACS Applied Materials & Interfaces*, **2016**, 8, 15524-15534.
7. Chen, Xian-Kai; Ravva, Mahesh Kumar; Li, Hong; **Ryno, Sean M.**; Brédas, Jean-Luc. "Effect of Molecular Packing and Charge Delocalization on Non-Radiative Recombination of Charge-Transfer States in Organic Solar Cells." *Advanced Energy Materials*, **2016**, 1601325.
8. **Ryno, Sean M.**; Ravva, Mahesh K.; Chen, XianKai; Li, Haoyuan; Brédas, Jean-Luc. "Molecular Understanding of Fullerene–Electron Donor Interactions in Organic Solar Cells." *Advanced Energy Materials*, *Accepted*, **2016**.

## PRESENTATIONS

1. "Electronic Polarization at Organic-Vacuum and Organic-Organic Interfaces" **S. M. Ryno**, C. Risko, and J. L. Brédas. Poster presented at the 2016 International Conference on Science and Technology of Synthetic Metals (June 26 – July 1, 2016), Guangzhou, China.
2. "Charge Polarization in Organic Electronic Materials: From Bulk Materials to Organic Interfaces" **S. M. Ryno**, C. Risko, and J. L. Brédas. Invited poster presentation at the International Symposium of Functional Materials (January 25-29, 2016), Okinawa Institute of Science and Technology, Okinawa, Japan.

3. "Charge Polarization in Organic Electronic Materials: From Bulk Materials to Organic Interfaces" **S. M. Ryno**, C. Risko, and J. L. Brédas. Poster presented at the 3<sup>rd</sup> Annual Solar Future Symposium (November 7-11, 2015), King Abdullah University of Science and Technology, Thuwal, Kingdom of Saudi Arabia.
4. "Employing Polarizable Force Fields to the Study of Charge Polarization in Organic Molecular Crystals." **S. M. Ryno**, C. Risko, and J. L. Brédas. Poster presented at the 2<sup>nd</sup> Annual Solar Future Symposium (November 8-11, 2014), King Abdullah University of Science and Technology, Thuwal, Kingdom of Saudi Arabia.
5. "Employing Polarizable Force Fields to the Study of Charge Polarization in Organic Molecular Crystals." **S. M. Ryno**, S. R. Lee, J. S. Sears, C. Risko, and J. L. Brédas. Poster presented at the 11<sup>th</sup> International Symposium on Functional  $\pi$ -Electron Systems (June 2-7, 2013), Arcachon, Aquitaine, France.
6. "Employing Polarizable Force Fields to the Study of Charge Polarization in Organic Molecular Crystals." **S. M. Ryno**, S. R. Lee, J. S. Sears, C. Risko, and J. L. Brédas. Poster presented at the 2012 International Conference on Science and Technology of Synthetic Metals (July 8-13, 2012), Atlanta, GA.
7. "Differential Scanning Calorimetric Study of a Thermochromic Anil." **S. M. Ryno** and D. Thompson. Poster presented at the 2010 Herty Medalist Undergraduate Research Symposium (September 17, 2010), Moorehouse College.

## COMPUTATIONAL SKILLS

- Proficient in the use of the Python and Bash scripting languages.
- Understanding of C, C++, and Fortran languages sufficient to reverse engineer or incorporate into Python.
- Extensively use Gaussian, GROMACS, QCHEM, PSI4, Molpro, VASP, MATLAB, Tinker, LAMMPS, Materials Studio, GDMA, and OriginPro software packages.

## Affiliations

- American Chemical Society, Member, 2015-Present

## REFERENCES

**Professor Jean-Luc Brédas** (PhD Advisor), Physical Science and Engineering  
King Abdullah University of Science and Technology, Thuwal, Kingdom of Saudi Arabia  
E-mail: Jean-Luc.Bredas@kaust.edu.sa

**Professor Chad Risko**, Department of Chemistry  
University of Kentucky, Lexington, Kentucky  
E-mail: Chad.Risko@uky.edu

**Professor Kenneth Brown**, School of Chemistry and Biochemistry

Georgia Institute of Technology  
E-Mail: [Ken.Brown@chemistry.gatech.edu](mailto:Ken.Brown@chemistry.gatech.edu)