Sean M. Ryno: Curriculum Vitae

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EDUCATION

Georgia Institute of Technology Atlanta, GA
Ph. D., Chemistry GPA: 3.42 August 2015
Research Advisor: Professor Jean-Luc Brédas
Thesis: Molecular-Scale Understanding of Electronic Polarization in Organic Molecular Crystals

University of North Georgia Dahlonega, GA
B.S., Chemistry GPA: 3.60 (Cum Laude) 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

Universal Display Corporation Ewing, NJ
Research Scientist 04/2018-Present
Research Manager: Doctor George Fitzgerald

- Applying various methodologies to advancing the understanding of organic light emitting devices.

University of Kentucky Lexington, KY
Post-Doctoral Scholar 11/2016-03/2018
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.
- Applying molecular dynamics to model crystal nucleation and growth to study the effect of grain boundaries on the materials characteristics of organic semiconductors.
- Parameterizing 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 Thuwal, KSA
Post-Doctoral Fellow / Student Researcher 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 Atlanta, GA
Teaching Assistant for Chemical Principles 1211K 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*, **2017**, 7, 1601370.
9. McDowell, Caitlin; Narayanaswamy, Kamatham; Yadagiri, Bommaramoni; Gayathri, Thumuganti; Seifrid, Martin; Datt, Ram; **Ryno, Sean M.**; Heifner, Michael C.; Gupta, Vinay; Risko, Chad; Singh, Surya Prakash; Bazan, Guillermo C. " Impact of Rotamer Diversity on the Self-Assembly of Nearly Isostructural Molecular Semiconductors." *Journal of Materials Chemistry A*, **2018**, 6, 386-394.

10. Abtahi, Ashkan; Mazza, Samuel M.; **Ryno, Sean M.**; Loya, E. Kirkbride; Li, Ruipeng; Parkin, Sean R.; Risko, Chad; Anthony, John E.; Graham, Kenneth R. "Effect of Halogenation on the Energetics of Pure and Mixed Phases in Model Organic Semiconductors Composed of Anthradithiophene Derivatives and C60." *The Journal of Physical Chemistry C*, **2018**, 122, 4757-4767.
11. Purdum, Geoffrey; Telesz, Nicholas G.; Jarolimek, Karol; **Ryno, Sean M.**; Gessner, Thomas; Davy, Nicholas C.; Petty II, Anthony; Zhen, Yonggang; Shu, Ying; Facchetti, Antonio; Collis, Gavin E.; Hu, Wenping; Wu, Chao; Anthony, John E.; Weitz, R. Thomas; Risko, Chad; Loo, Yueh-Lin. "Presence of Short Intermolecular Contacts Screens for Kinetic Stability in Packing Polymorphs." *Journal of the American Chemical Society*, **2018**, 140, 7519-7525.
12. Li, Shi; **Ryno, Sean M.**; Risko, Chad. "Exploring Thermal Transitions in Anthradithiophene-Based Organic Semiconductors to Reveal Structure-Packing Relationships." *Journal of Materials Chemistry C*, **2018**, Advance Article.

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 3rd 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 2nd 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 11th International Symposium on Functional π-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 Calormetric 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.
- Extensive use of the Gaussian, GROMACS, QCHEM, PSI4, Molpro, VASP, MATLAB, Tinker, LAMMPS, Materials Studio, GDMA, SCHRODINER, 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