Davita L. Watkins, Ph.D.

University of Mississippi, Department of Chemistry and Biochemistry
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Education

Doctorate of Philosophy, Chemistry — Memphis, TN
The University of Memphis — 2007-2012
Dissertation: *Novel Photochromic Spirooxazine Dimers: Synthesis, Characterization, and Applications*

Bachelor of Science, Chemistry and Anthropology — Nashville, TN
Vanderbilt University — 2002-2006

Employment History

Assistant Professor of Chemistry — University, MS
The Watkins Laboratory, University of Mississippi — 2014-present

- Optoelectronic behavior of halogen bond assemblies as semiconducting materials; self-assembling Janus dendrimers and linear–dendritic block copolymers for theranostics
  - *Collaborative studies* – calmodulin-based biomaterials; anti-cancer agents derived from panobinostat; self-assembling magnesium oxide (MgO_2) nanoparticles; electro-copolymerization
  - *Thesis/Dissertation Advising* – Jon Steven Dal Williams, Briana Simms, Dilan Karunathilaka, Mahesh De Silva, Sajith Vijayan, Indika Chandrasiri, Tharindu Ranathunge, Nicholas Sparks, Blaine Derbigny
  - *Postdoctoral Advising* – Daniel G. Abebe and Sivaraman Balasubramaniam

Postdoctoral Research Associate — Gainesville, FL
The Castellano Laboratory, University of Florida — 2012-2014

- Self-assembling oligomers for photovoltaic devices; solution and solid phase characterization of assembly formation, optoelectronic properties and redox behavior of semiconductors
  - *Advisor* – Dr. Ronald K. Castellano, Professor of Chemistry

Graduate Research Assistant — Memphis, TN
The Fujiwara Laboratory, University of Memphis — 2007-2012

- Photochromic compounds and polymer systems for selective recognition of biomolecules and sensoring of organic/inorganic molecules
  - *Advisor* – Dr. Tomoko Fujiwara, Associate Professor of Chemistry

Chemical Analyst I — Memphis, TN
Eurofins Scientific Incorporated, Memphis Division — 2006-2007

Monsanto Summer Intern — Memphis, TN
Agriculture Company, Memphis Division — 2006-2006

Undergraduate Researcher — Nashville, TN
The Hercules Laboratory, Vanderbilt University — 2005-2006

- Characterization of decomposition occurring in polystyrene based systems via MALDI-TOF mass spectrometry
  - *Advisor(s)* – Dr. David Hercules, Professor of Chemistry

and Dr. Grace Zoorob, Professor of Chemistry

Awards

2018 International Symposium on Halogen Bonding Rising Star 2018
- Invited speaker

2018 Emerging Investigators - Journal of Materials Chemistry C 2018
- Faculty early career journal issue

Mike L. Edmonds New Scholar Award 2018
- UM faculty early career development award

American Chemical Society Young Investigator Award 2018
- PMSE faculty early career award

Lloyd N. Ferguson Young Scientist Award for Excellence in Research 2018
- NOBCChE faculty early career award

National Science Foundation CAREER Award 2017

Oak Ridge Associated Universities (ORAU) Ralph E. Powe Award 2015

Carl Storm Underrepresented Minority (CSURM) Fellowship 2013
- Financial support to attend the 2013 Physical Organic Chemistry Gordon Research Conference; selected speaker

5th Annual National Science Foundation (NSF) Future Faculty Workshop 2012
- Selected and invited scholar

Dow Chemical Company B. E. S. T. Symposium, Invited scholar 2012

First Generation Ph.D. Scholar, Fellowship recipient 2008-2012

Service

Member at Large American Chemical Society PMSE Division 2019

Sigma Xi Scientific Research Honor Society, Member 2019

National Science Foundation (NSF) Future Faculty Mentor 2018

Operation ICB (I Can Be), Program coordinator 2015

University Chapter of the National Organization of Black Chemist and Chemical Engineers (NOBCChE), UM co-advisor 2015

Society of STEM Women of Color, Inc., Member 2015

Local Section American Chemical Society (ACS) Governance, Secretary 2014-2017

American Chemical Society (ACS), Member 2012

Publications*

Sparks, N.; Ranathunge, T. A.; Karunathilaka, D.; Tate, C. M.; Delcamp, J. H.; Rajapakse, R. M. G.; and **Watkins, D. L.** "Achieving Complex Isoindigo-based Donor-Acceptor (D–A) Type Copolymeric Materials Via Electro-Copolymerization," ChemElectroChem, 2020, *submitted.*

Yaddehige, M. L.; Chandrasiri, I.; Kotha, A.; Barker, A.; Simms, B. L.; Williams, J. S. D.; Abebe, D. G.; Kucheryavy, P.; Chougule, M. B.; and **Watkins, D. L.** "Cationic, Anionic and Neutral Functionalized PAMAM - Fatty Acid Amphiphilic Janus Dendrimers for Therapeutic Applications," Org. Biomol. Chem., 2020, *submitted.*

Chandrasiri, I.; Abebe, D. G.; Yaddehige, M. L.; Williams, J. S. D.; Zia, M. F.; Dorris, A.; Barker, A.; Simms, B. L.; Parker, A.; Le, N.; Gayton, J. N.; Hammer, N. I.; Flynt, A.; Delcamp, J. H.; and **Watkins, D. L.**, "Self-Assembling PCL-PAMAM Linear Dendritic

Block Copolymers (LDBCs) for Bioimaging and Phototherapeutic Applications," ACS Appl. Bio Mater., 2020, *submitted.*

Ranathunge, T. A.; Ngo, D.; Karunathilaka, D.; Attanayake, N. H.; Chandrasiri, I.; Delcamp, J. H.; Rajapakse, R. M. G.; and **Watkins, D. L.** "Hierarchical Structures of Complex Electronically Conducting Organic Polymers Via One-Step Electro-Polymerization," J. Mater. C., 2020, DOI: 10.1039/c9tc06945c

Balasubramaniam, S.; May, X., Rivas, F., Dodson, K., Vijayan, S. Adhikari, S., **Watkins, D. L.**, Stoddard, S. "Design and Synthesis of Diazine-based Panobinostat Analogues for HDAC8 Inhibition," Beilstein J. Org. Chem., 2020, 16, 628–637, DOI:10.3762/bjoc.16.59

Stoddard, S. V., Dodson, K., Adams, K., **Watkins, D. L.**, "In silico Design of Novel Histone Deacetylase 4 Inhibitors: Design Guidelines for Improved Binding Affinity," Int. J. Mol. Sci. 2020, DOI: 10.3390/ijms21010219

Ranathunge, T. A.; Ngo, D.; Attanayake, N. H.; Karunathilaka, D.; Delcamp, J. H.; Rajapakse, R. M. G.; and **Watkins, D. L.** "Radically Accessing D–A Type Ambipolar Copolymeric Materials with Intrinsic Electrical Conductivity and Visible–Near Infrared Absorption Via Electro-Copolymerization," Macromol. Chem. Phys., 2019, 220, 1900289, DOI: 10.1002/macp.201900289

Steen, A. E., Ellington, T. L., Shuford, K. L., Tschumper, G. S., **Watkins, D. L.** and Hammer, N. I. "A Raman Spectroscopic and Computational Study of New Aromatic Pyrimidine-Based Halogen Bond Acceptors," Inorganics: Special Issue on Halogen Bonding, 2019, 7(10), 119, DOI: 10.3390/inorganics7100119

Steen, A; Ellington, T. L.; Nguyen, S. T.; Balasubramaniam, S.; Chandrasiri, I.; Delcamp, J. H.; Tschumper, G. S.; Hammer, N. I.; **Watkins, D. L.** "Probing the Photophysical Behavior of Furan- and Thiophene-Containing Bispyridyl Oligomers via Spectroscopic and TD-DFT Methods," J. Phys. Chem. C. 2019, DOI: 10.1021/acs.jpcc.9b01510

Chandrasiria, I.; Abebe, D. G.; Gupta, S.; Williams, J. S. D.; Rieger, W. D.; Simms, B. L.; Noh,Y.; Payne, M. E.; Fortenberry, A.; Smith, A.; Lee, B.; Grayson, S. M.; Schneider, G. J. and **Watkins, D. L.**, "Synthesis and Characterization of PAMAM-Polylactide "Janus-type" Linear-Dendritic Hybrids." J. Polym. Sci. A, 2019, DOI: 10.1002/pola.29409

Johnson, S. N.; Ellington, T. L.; Nevarez, J.; Ngo, D.; Sparks, N.; Rheingold, A. L.; **Watkins, D. L.** and Tschumper, G. S. "Probing Non-covalent Interactions Driving Molecular Assembly in Organo-electronic Building Blocks," CrystEngComm., 2019, DOI: 10.1039/C9CE00219G.

Rajapakse, R. M. G.; Attanayake, N. H.; Karunathilaka, D.; Steen, A. E., Hammer, N. I.; Strongin, D. R.; and **Watkins, D. L.** "Advances in Electro-copolymerization of NIR Emitting and Electronically Conducting Block Copolymers" J. Mater. C. (Communications), 2019, DOI: 10.1039/C8TC06331A

Ranathunge, T. A.; Karunaratne, D.; Rajapakse, R.; **Watkins, D.L.** "Doxorubicin Loaded Magnesium Oxide Nanoflakes as pH Dependent Carriers for Simultaneous Treatment of Cancer and Hypomagnesemia," Nanomaterials., 2019, DOI: 10.3390/nano9020208

May, X., Rivas, F., Dodson, K., Vijayan, S. Adhikari, S., Parker, K., **Watkins, D. L.**, Stoddard, S. "Design of Potent Panobinostat Histone Deacetylase Inhibitor Derivatives: Molecular Considerations for Enhanced Isozyme Selectivity between HDAC2 and HDAC8," Mol. Inf., 2018, DOI:10.1002/minf.201800080

Baumann, A., Cheema, H., Sabuj, M A., McNamara, L. E., Peddapuram, A., Zhang, Y., Nguyen, S. T., **Watkins, D. L.**, Hammer, N. I., Raib, N. and Delcamp, J. H. "Iodine Binding with Thiophene Versus Furan Based Dyes for DSC," Phys. Chem. Chem. Phys. 2018, DOI: 10.1039/c8cp03065k

Weldeab, A. O.; Starkenburg, D. J.; Steen, A., Abboud, K. A.; Xue, J.; Castellano, R. K.; and **Watkins, D. L.**. "Hierarchical Assembly of a Low Energy Gap π-Conjugated Oligomer via Synergetic Halogen and Hydrogen Bonding," J. Mater. Chem. C. 2018, DOI: 10.1039/c8tc00074c

Nguyen, S. T., Ellington, T. L., Allen, K. E., Gorden, J. D., Rheingold, A. L., Tschumper, G. S., Hammer, N. I., and **Watkins, D. L.** "Systematic Experimental and Computational Studies of Substitution and Hybridization Effects in Solid-State Halogen Bonded Assemblies," Cryst. Growth Des., 2018, DOI: 10.1021/acs.cgd.8b00398

Cheema, H.; Peddapuram, A.; Adams, R.; McNamara, L.; Hunt, L.; Le, N.; **Watkins, D. L.**; Hammer, N. I.; Schmehl, R.; Delcamp, J. "Molecular Engineering of NIR Absorbing Thienopyrazine Double Donor Double Acceptor Organic Dyes for DSCs". J. Org. Chem. 2017, DOI: 10.1021/acs.joc.7b01750.

Zhang, Y.; Autry, S.; McNamara, L.; Nguyen, S.; Le, N.; Brogdon, P.; **Watkins, D. L.**; Hammer, N.I.; Delcamp, J. "Near-Infrared Fluorescent Thienothiadiazole Dyes with Large Stokes Shifts and High Photostability", J. Org. Chem. 2017, DOI: 10.1021/acs.joc.7b00422

Gindt, B. P.; Tang, Z.; **Watkins, D. L.**; Abebe, D. G.; Seo, S.; Tuli, S.; Ghassemi, H.; Zawodzinski, T. A.; Fujiwara, T. "Effects of Sulfonated Side Chains Used in Polysulfone-based PEMs for VRFB Separator", J. Membrane Sci. 2017, DOI: 10.1016/j.memsci.2017.03.013.

Ellington, T.L.; Reves, P.L.; Simms, B.L.; Wilson, J.L.; **Watkins, D. L.**; Tschumper, G.S.; Hammer, N.I. "Quantifying the Effects of Halogen Bonding by Haloaromatic Donors on the Acceptor Pyrimidine", Phys. Chem.Chem. Phys. 2017, DOI: 10.1002/cphc.201700114

Nguyen, S.T.; Rheingold, A.; Tschumper, G. S.; **Watkins, D. L.** "Elucidating the Effects of Fluoro and Nitro Substituents on Halogen Bond Driven Assemblies of Pyridyl-capped π-Conjugated Molecules", Cryst. Growth Des. 2016, DOI: 10.1021/acs.cgd.6b01321

Albers, T.; **Watkins, D. L.**; Gameiro, A.; Povstyanoy, V. y.; Povstyanoy, M.; Lebedyeva, I., Benzotriazole-Based Strategies Toward Peptidomimetics, Conjugates, and Other Peptide Derivatives. In Topics in Heterocyclic Chemistry, Springer Berlin Heidelberg: 2015; 1-47.

Wilson, J.; Williams, J. S. D.; Petkovsek, C.; Reves, P.; Jurss, J. W.; Hammer, N. I.; Tschumper, G. S.; **Watkins, D. L.** "Synergistic Effects of Halogen Bond and π-π Interactions in Thiophene-based Building Blocks", R. Soc. Chem. Adv. 2015, DOI: 10. 1039/C5RA16680B.

Shewmon, N. T.; **Watkins, D. L.**; Galindo, J.; Bou Zerdan, R.; Chen, J.; Keum, J.; Roitberg, A. E.; Xue, J.; Castellano, R. K. "Enhancement in Organic Photovoltaic Efficiency through the Synergistic Interplay of Molecular Donor Hydrogen Bonding and π-Stacking", Adv. Funct. Mater. 2015, 25, 5166-5177. DOI: 10.1002/adfm.201501815

Xueying, Z.; Cruz, J. F.; **Watkins, D. L.**; Xue, J.; Roitberg, A. E.; Castellano, R. K.; Perry, S. S. "Hydrogen Bond Directed Assembly of Oligothiophene/fullerene Superstructures on Au", Org. Electron. 2015, 19, 61-69. DOI: 10.1016/j.orgel.2015.01.022

Schulze, B. M.; **Watkins, D. L.**; Zhang, J.; Ghiviriga, I.; Castellano, R. K. "Estimating the Shape and Size of Supramolecular Assemblies by Variable Temperature Diffusion Ordered Spectroscopy", Org. Biomol. Chem. 2014, 12, 7932-7936. DOI: 10.1039/C4OB01373E

Schulze, B. M.; Shewmon, N. T.; Zhang, J.; **Watkins, D. L.**; Mudrick, J. P.; Cao, W.; Bou Zerdan, R.; Quartararo, A. J.; Ghiviriga, I.; Xue, J.; Castellano, R. K. "Consequences of Hydrogen Bonding on Molecular Organization and Device Performance in Molecular Organic Photovoltaic Cells", J. Mater. Chem. A. 2014, 2, 1541-1549. DOI: 10.1039/C3TA13529B

Watkins, D. L.; Fujiwara, T. "Bis-Spironaphthooxazine Based Photochromic Polymer Materials", J. Mater. Chem. C. 2013, 1, 506-514. DOI: 10.1039/C2TC00098A

Watkins, D. L.; Fujiwara, T. "Synthesis, Characterization, and Solvent-Independent Photochromism of Spironaphthooxazine Dimers", J. Photochem. Photobiol. A: Chem. 2012, 228, 51-59.

Kumar, S.; **Watkins, D. L.**; Fujiwara, T. "Tailored Spirooxazine Dimer as a Photoswitchable Binding Tool", Chem. Commun. 2009, 28, 4369-4371.

***Total publications: 33; over 50 oral and poster presentations**

Funding

Oak Ridge Associated Universities (ORAU): Ralph E. Powe Junior Faculty Enhancement Award, Halogen Bond Driven Self-Assembly of Hybrid Oligomers for Organic Semiconducting Devices (PI); TOTAL: $10,000

National Science Foundation: CAREER: Elucidating the Role of Sigma-hole Interactions in Advanced Functional Materials (PI); TOTAL: $493,549; Award Abstract #1652094

National Science Foundation: Mississippi NSF EPSCoR RII-Track 1: Center for Emergent Molecular Optoelectronics (CEMOs) (Thrust Leader); TOTAL: $20,000,000; Award Abstract #1757220

National Science Foundation: Mississippi NSF EPSCoR RII Track-2 FEC. Collaborative Research and Education on Synergized Transformational Solar Chemical Looping and Photo-Ultrasonic Renewable Biomass Refinery (Senior Personnel); TOTAL: $ 1,600,000; Award Abstract #1632899

American Chemical Society Petroleum Research Fund New Directions: Elucidating the Effects of Molecular Structure on Janus Dendrimers as Ambidextrous Gelators (PI); TOTAL: $110,000; recommended for funding