# Eric Van Dornshuld, Ph.D.

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EXPERIENCE	
Mississippi State University, Mississippi State, MS Assistant Clinical Professor Instructor Post-Doctoral Teaching/Research Associate	2018–present 2017–2018 2014–2017
<b>The University of Mississippi, University, MS</b> Research Assistant Teaching Assistant	2009–2014 2009–2010
The University of North Florida, Jacksonville, FL Research Assistant Teaching Assistant	2006–2009 2007–2008
EDUCATION	
<b>Ph.D. Chemistry</b> The University of Mississippi, University, MS Dissertation: "Characterizing non-covalent interactions and peptide bond formation with electronic structure theory" Advisor: Prof. Gregory S. Tschumper	August 2014
<b>B.S. Chemistry</b> The University of North Florida, Jacksonville, FL Advisor: Prof. Robert Vergenz (retired)	May 2009
AWARDS	
ChemDawg Recognition Award	2020
for "Outstanding effort and contributions to the Department of Chemistry" MS ACS Local Section – ACS ChemLuminary Award for "Best National Chemistry Week Event Organized By a Student Group"	2019
MS ACS Local Section – ACS Student Chapter of the Year (SMACS)	2018
ACS Graduate Research Award	2014 2014
Dissertation Fellowship Award	2014
GRANTS	
ACS Innovative Project Grant	2019

## PUBLICATIONS

- 1. Olive, L. N., E. V. Dornshuld and C. E. Webster. The curious case of DMSO: A CCSD(T)/CBS(aQ56+d) benchmark and DFT study J. Chem. Phys. 2021. 114304, doi:10.1002/jcc.23522
- 2. Frey, N. C., E. V. Dornshuld and C. E. Webster. Benchmarking the Fluxional Processes of Organometallic Piano-Stool Complexes *Molecules*. 2021. 26, 2310, doi:10.3390/molecules26082310
- 3. Bhavsar-Jog, Y., E. V. Dornshuld, T.A. Brooks, G. S. Tschumper, and R. M. Wadkins. Co-Localization of DNA i-Motif-Forming Sequences and 5-Hydroxymethyl-cytosines in Human Embryonic Stem Cells. Molecules. 2019. 24, 3619, doi:10.3390/molecules24193619.
- 4. Dornshuld, E. V. and G. S. Tschumper. Big Changes for Small Noncovalent Dimers: Revisiting the Potential Energy Surfaces of  $(P_2)_2$  and  $(PCCP)_2$  with CCSD(T) Optimizations and Vibrational Frequencies. J. Chem. Theory Comput. 2016. 12, 4, 1534–1541, doi:10.1021/acs.jctc.5b01105.

- 5. Dornshuld, E. V., R. A. Vergenz, and G. S. Tschumper. Peptide bond formation via glycine condensation in the gas phase. *J. Phys. Chem. B.* **2014**. *118* (29), 8583–8590, doi:10.1021/jp504924c.
- Dornshuld, E. V., C. M. Holy and G. S. Tschumper. Homogeneous and heterogeneous non-covalent dimers of formaldehyde and thioformaldehyde: structures, energetics, and vibrational frequencies. J. Phys. Chem. A. 2014. 118 (18), 3376–3385, doi:10.1021/jp502588h.
- Bhavsar-Jog, Y., E. V. Dornshuld, T.A. Brooks, G. S. Tschumper, and R. M. Wadkins. Epigenetic modification, dehydration, and molecular crowding effects on the thermodynamics of i-motif structure formation from C-rich DNA. *Biochemistry*. **2014**. *53* (10), 1586–1594, doi:10.1021/bi401523b.
- Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of two small but challenging noncovalent dimers: (P<sub>2</sub>)<sub>2</sub> and (PCCP)<sub>2</sub>. *J. Comput. Chem.* **2014**. *35* (6), 479–487, doi:10.1002/jcc.23522.
- Reddy, V., R. Kota, E. V. Dornshuld, D. L. Mattern, G. S. Tschumper, D. Jiang, and A. Dass. Interstaple dithiol cross-linking in Au<sub>25</sub>(SR)<sub>18</sub> nanomolecules: a combined mass spectrometric and computational study. *J. Am. Chem. Soc.*. 2011. 133 (50), 20258–20266, doi:10.1021/ja206436x.
- 10. Dornshuld, E. V., M. Zhang, T. Keith Hollis, and C. E. Webster. Predicting <sup>195</sup>Pt-NMR chemical shifts in organometallic compounds with non-relativistic density functional approaches. (in preparation)

#### **TEACHING EXPERIENCE**

CH-1213 – Chemistry I	CH-3141 – Prof. Chem: Literature
CH-1223 – Chemistry II	CH-4711 – Senior Seminar
CH-1141 – Prof. Chem: Paths	CH-8990 – Prof. Chem: Current Problems (compu-
CH-2141 – Prof. Chem: Tools	tational chemistry project support)
SERVICE	
DEPARTMENT	
Department of Chemistry Website Manager	2018–2020
Undergraduate Curriculum Committee Member	2020-present
Undergraduate Curriculum Development	2017-present
Faculty Advisor to the MSU SMACS	2016-present
College	
College of Arts & Sciences Scholarship Committee	2018–2021
PROFESSIONAL	
National Chemistry Week Coordinator (MS Local AC	S Section) 2019–present
AUTHORED CURRICULUM	
Investigations in Chemistry II CH-1221 Lab Manual,	1st ed. 2021
T. Brown, Dornshuld, E. V., W. Nettles, and C. E. V	
CH-1213 Chemistry I Coursebook, 4th ed.	
Dornshuld, E. V., W. Nettles, and C. E. Webster	
CH-1223 Chemistry II Coursebook, 5th ed.	
Dornshuld, E. V., W. Nettles, and C. E. Webster	
CH-1213 Chemistry I Workbook, 3rd ed.	2020
Dornshuld, E. V., W. Nettles, and C. E. Webster	
CH-1223 Chemistry II Workbook, 4th ed.	
Dornshuld, E. V., W. Nettles, and C. E. Webster	
CH-1213 Chemistry I Workbook, 2nd ed.	2019
Dornshuld, E. V., W. Nettles, and C. E. Webster	
CH-1223 Chemistry II Workbook, 3rd ed.	
Dornshuld, E. V., W. Nettles, and C. E. Webster	
CH-1213 Chemistry I Workbook, 1st ed.	2018

Dornshuld, E. V., W. Nettles, and C. E. Webster CH-1223 Chemistry II Workbook, 2nd ed. Dornshuld, E. V., W. Nettles, and C. E. Webster CH-1223 Chemistry II Workbook, 1st ed. Dornshuld, E. V.

## **ORAL PRESENTATIONS**

- Dornshuld, E. V., M. Zhang, T. K. Hollis, and C. E. Webster. Characterizing <sup>195</sup> Pt NMR chemical shift with computationally tractable non-relativistic density functional approaches. 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, November 7–11, 2017.
- 2. Dornshuld, E. V. Computational Chemistry: A Primer (or what you should know when you want have to talk to a computational chemist). *Feeding and Powering the World*, University, MS, June 19, 2017.
- Dornshuld, E. V., M. Zhang, T. K. Hollis, and C. E. Webster. Utilizing computational <sup>195</sup>Pt NMR chemical shifts for the prediction of meridional ligand donor ability in square planar complexes. *Feeding and Powering the World 2016: Building the Network*, University, MS, July 25–26, 2016
- Dornshuld, E. V., R. A. Vergenz, R. Mourad, M. A. Carrasquillo, J. W. Vickers, and H. F. Schaefer. Mechanism for aqueous glycine condensation. 2008 ACS 236th National Meeting, Philadelphia, PA, August 17–20, 2008.

## WORKSHOPS

1. Telluride School on Theoretical Chemistry (TSTC)

July 15–20, 2013

2017

# POSTER PRESENTATIONS

- Dornshuld, E. V., M. Zhang, X. Zhang, T. K. Hollis, and C. E. Webster. Predicting <sup>195</sup>Pt NMR chemical shifts in small Pt(II) and Pt(IV) organometallic compounds with density functional approaches. 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, November 4–7, 2015.
- 2. Dornshuld, E. V., C. M. Holy, and G. S. Tschumper. New insight into  $n \rightarrow \pi^*$  non-covalent interactions from two simple systems, formaldehyde dimer and thioformaldehyde dimer. *Mississippi Experimental Program to Stimulate Competitive Research State Meeting (EPSCoR)*, April 1, 2014.
- 3. Dornshuld, E. V., C. M. Holy, and G. S. Tschumper. New insight into  $n \rightarrow \pi^*$  non-covalent interactions from two simple systems, formaldehyde dimer and thioformaldehyde dimer. *25th Austin Symposium on Molecular Structure and Dynamics (ASMD@D)*, March 1–4, 2014.
- Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the P<sub>2</sub> dimer and the PCCP dimer. *Southeast Theoretical Chemistry Association Annual Meeting (SETCA 2013)*, May 9–11, 2013.
- Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the P<sub>2</sub> dimer and the PCCP dimer. *Mississippi Experimental Program to Stimulate Competitive Research State Meeting (EPSCoR)*, April 18, 2013.
- Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the P<sub>2</sub> dimer and the PCCP dimer. *53rd Sanibel Symposium*, February 17–22, 2013.
- Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the P<sub>2</sub> dimer and the PCCP dimer. *Mississippi Experimental Program to Stimulate Competitive Research Fall Forum* (EPSCoR), August 28, 2012.
- Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the P<sub>2</sub> and PCCP dimers. *Southeast Theoretical Chemistry Association Annual Meeting (SETCA 2012)*, May 17–19, 2012.
- Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the P<sub>2</sub> and PCCP dimers. *Mississippi Experimental Program to Stimulate Competitive Research State Meeting*, April 10, 2012.

- 10. Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the P<sub>2</sub> and PCCP dimers. *Mississippi Experimental Program to Stimulate Competitive Research Fall Forum* (*EPSCoR*), September 20, 2011.
- 11. Dornshuld, E. V. and G. S. Tschumper. The molecular structures of the P<sub>2</sub> and PCCP dimers. *Southeast Theoretical Chemistry Association Annual Meeting (SETCA 2011)*, May 13–14, 2011.
- 12. Dornshuld, E. V. and G. S. Tschumper. The molecular structures of the P<sub>2</sub> and PCCP dimers. *Mississippi Experimental Program to Stimulate Competitive Research State Meeting (EPSCoR)*, April 14, 2011.
- Dornshuld, E. V., R. A. Vergenz, H. F. Schaefer, III, and G. S. Tschumper. Exploring the stepwise mechanism of aqueous glycine condensation. 19th Conference on Current Trends in Computational Chemistry (CCTCC 2010), October 29–30, 2010.
- 14. Dornshuld, E. V., R. A. Vergenz, H. F. Schaefer, III, and G. S. Tschumper. Exploring the mechanism for aqueous glycine condensation. *Mississippi Experimental Program to Stimulate Competitive Research State Meeting (EPSCoR)*, April 15, 2010.
- 15. Dornshuld, E. V., R. A. Vergenz, and R. Mourad. Mechanism for aqueous glycine condensation. *48th Sanibel Symposium*, February 21–26, 2008.
- 16. Bruno, P., M. Carrasquillo, N. Durtshi, E. V. Dornshuld, and J. Vickers. Do weak methyl-donated hydrogen bonds affect protein folding and stability? *Colorado Protein Stability Conference*, July 19, 2007.

#### **CONTRIBUTED PRESENTATIONS**

- 1. Olive, L., E. V. Dornshuld, and C. E. Webster. Curious case of DMSO: A computational study. *52nd Southeastern Undergraduate Research Conference*, Tuscaloosa, AL, January 25, 2020.
- Olive, L., E. V. Dornshuld, and C. E. Webster. Curious case of DMSO: A computational study. 258th ACS National Conference and Exposition, San Diego, CA, August 25–29 2019.
- Olive, L., E. V. Dornshuld, and C. E. Webster. New insights into assessing the performance of DFT energetics on small oxygen/sulfur containing compounds. *Summer Undergraduate Research Symposium*, Mississippi State, MS, August 2019.
- Olive, L., E. V. Dornshuld, and C. E. Webster. Assessing the performance of DFT energetics on small oxygen/sulfur containing compounds. *Feeding and Powering the World 2019: The Next Generation*, University, MS, July 15–16, 2019.
- Frey, N. C., E. V. Dornshuld, F. Aghabozorgi, and C. E. Webster. Characterizing the fluxional behavior in (TMCOT)M(CO)<sub>3</sub> and (COT)Cr(CO)<sub>3</sub> complexes with computational approaches. *Feeding and Powering the World 2019: The Next Generation*, University, MS, July 15–16, 2019.
- Frey, N. C., E. V. Dornshuld, F. Aghabozorgi, and C. E. Webster. Examining the electronic properties of twisted pyrene compounds. *Feeding and Powering the World 2019: The Next Generation*, University, MS, July 15–16, 2019.
- Autry, S., M. Zhang, E. V. Dornshuld, T. K. Hollis, and C. E. Webster. Probing the effects of environment on novel CCC-NHC-Pt(II) pincer complexes. 257th ACS National Meeting and Exposition, Orlando, FL Mar. 31 – Apr. 4, 2019.
- Zhang, M., E. V. Dornshuld, J. C. Bunquin, M. Delferro, T. K. Hollis, and C. E. Webster. The platinum electronic parameter (PtEP): A compliment to TEP. *Feeding and Powering the World 2018: Planning for the Future*, University, MS, July 16–17, 2018.
- Adiraju, K., M. Zhang, E. V. Dornshuld, R. W. Lamb, G. Liang, C. E. Webster, and T. K. Hollis. State-ofthe-art nitrogen reduction: Haber-Bosch to homogeneous back to heterogeneous. *Feeding and Powering the World 2018: Planning for the Future*, University, MS, July 16–17, 2018.
- Zhang, M., S. Autry, V. Dixit, E. V. Dornshuld, J. Denny, N. Hammer, C. E. Webster and T. K. Hollis. Synthesis, characterization, and photophysics of CCC-NHC pincer platinum complexes. 255th ACS National Meeting and Exposition, New Orleans, LA, March 18–22, 2018.
- 11. Dixit, V., E. V. Dornshuld, C. E. Webster, and T. K. Hollis. Theoretical study of substituted CCC-NHC palladium and platinum complexes for OLED applications. *255th ACS National Meeting and Exposition*, New Orleans, LA, March 18–22, 2018.

- Hollis, T. K., C. E. Webster, M. Zhang, E. V. Dornshuld, V. Dixit, J. C. Bunquin, and M. Delferro. NHC pincer complex donor ability-PtEP (Platinum (Pt) electronic parameter): A donicity scale incorporating strictly meridional, tridentate ligands. *255th ACS National Meeting and Exposition*, New Orleans, LA, March 18–22, 2018.
- Hollis, T. K., C. E. Webster, M. Zhang, E. V. Dornshuld, J. C. Bunquin, and M. Delferro. NHC pincer complex donor ability? PtEP (platinum (Pt) electronic parameter): A donicity scale incorporating strictly meridional tridentate ligands. 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, November 7–11, 2017.
- V. Dixit, M. Zhang, E. V. Dornshuld, T. K. Hollis, C. E. Webster. Theoretical study of the effect of substituents on the optical spectra and <sup>195</sup>Pt NMR shift of CCC-NHC Pt(II) complexes. 69th Southeastern Regional Meeting of the American Chemical Society, Charlotte, NC, November 7–11, 2017.
- Zhang, M., E. V. Dornshuld, V. Dixit, J. A. Denny, C. E. Webster, and T. K. Hollis. Synthesis and characterization of CCC-NHC pincer platinum complexes. *Feeding and Powering the World 2016: Building the Knowledge Base*, University, MS, July 19–20, 2017.
- Dixit, V. E. V. Dornshuld, and C. E. Webster. Substitution effects on the emission spectra of platinum CCC-NHC pincer complexes. *Feeding and Powering the World 2016: Building the Network*, University, MS, July 25–26, 2016.
- Zhang, M., E. V. Dornshuld, X. Zhang, and C. E. Webster. Predicting metal complex reactivity for energy applications: Donicity of meridional tridentate ligands: <sup>195</sup>Pt NMR of CCC-NHC Pt pincer square planar complexes. *Feeding and Powering the World 2016: Building the Network*, University, MS, July 25–26, 2016.
- Lamb, R. W., E. V. Dornshuld, and C. E. Webster. Computational investigation of linkage isomerization in sulfoxide-containing ruthenium complexes. 67th Southeast/71st Southwest Joint Regional Meeting of the American Chemical Society, Memphis, TN, November 4–7, 2015.