

## Eric Van Dornshuld, Ph.D.

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### EXPERIENCE

#### Mississippi State University, Mississippi State, MS

Assistant Clinical Professor	2018–present
Instructor	2017–2018
Post-Doctoral Teaching/Research Associate	2014–2017

#### The University of Mississippi, University, MS

Research Assistant	2009–2014
Teaching Assistant	2009–2010

#### The University of North Florida, Jacksonville, FL

Research Assistant	2006–2009
Teaching Assistant	2007–2008

### EDUCATION

<b>Ph.D. Chemistry</b>	The University of Mississippi, University, MS	August 2014
Dissertation: “Characterizing non-covalent interactions and peptide bond formation with electronic structure theory”		
Advisor: Prof. Gregory S. Tschumper		

<b>B.S. Chemistry</b>	The University of North Florida, Jacksonville, FL	May 2009
Advisor: Prof. Robert Vergenz (retired)		

### AWARDS

MS ACS Local Section – ACS ChemLuminary Award	2019
for “ <i>Best National Chemistry Week Event Organized By a Student Group</i> ”	
MS ACS Local Section – ACS Student Chapter of the Year (SMACS)	2018
ACS Graduate Research Award	2014
Dissertation Fellowship Award	2014

### GRANTS

ACS Innovative Project Grant	2019
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### PUBLICATIONS

1. Olive, L., E. V. Dornshuld and C. E. Webster. The curious case of DMSO: A CCSD(T)/CBS benchmark study. (in preparation)
2. 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.
3. Dornshuld, E. V. and G. S. Tschumper. Big Changes for Small Noncovalent Dimers: Revisiting the Potential Energy Surfaces of (P<sub>2</sub>)<sub>2</sub> and (PCCP)<sub>2</sub> with CCSD(T) Optimizations and Vibrational Frequencies. *J. Chem. Theory Comput.* **2016**. *12*, 4, 1534–1541, doi:10.1021/acs.jctc.5b01105.
4. 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:  $(P_2)_2$  and  $(PCCP)_2$ . *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  $Au_{25}(SR)_{18}$  nanomolecules: a combined mass spectrometric and computational study. *J. Am. Chem. Soc.* **2011**. 133 (50), 20258–20266, doi:10.1021/ja206436x.
- Dornshuld, E. V., M. Zhang, T. Keith Hollis, and C. E. Webster. Predicting  $^{195}\text{Pt}$ -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 (computational chemistry project support)
CH-2141 – Prof. Chem: Tools	

## SERVICE

### DEPARTMENT

Department of Chemistry Website Manager	2018–present
Undergraduate Curriculum Development	2017–present
Faculty Advisor to the MSU SMACS	2016–present

### COLLEGE

College of Arts & Sciences Scholarship Committee	2018–present
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### PROFESSIONAL

National Chemistry Week Coordinator (MS Local ACS Section)	2019–present
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## AUTHORED CURRICULUM

<i>CH-1213 Chemistry I Workbook, 2nd ed.</i> Dornshuld, E. V., W. Nettles, and C. E. Webster	2019
<i>CH-1223 Chemistry II Workbook, 3rd ed.</i> Dornshuld, E. V., W. Nettles, and C. E. Webster	
<i>CH-1213 Chemistry I Workbook, 1st ed.</i> Dornshuld, E. V., W. Nettles, and C. E. Webster	2018
<i>CH-1223 Chemistry II Workbook, 2nd ed.</i> Dornshuld, E. V., W. Nettles, and C. E. Webster	
<i>CH-1223 Chemistry II Workbook, 1st ed.</i> Dornshuld, E. V.	2017

## ORAL PRESENTATIONS

- Dornshuld, E. V., M. Zhang, T. K. Hollis, and C. E. Webster. Characterizing  $^{195}\text{Pt}$  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.
- 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.

3. Dornshuld, E. V., M. Zhang, T. K. Hollis, and C. E. Webster. Utilizing computational  $^{195}\text{Pt}$  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
4. 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

## POSTER PRESENTATIONS

1. Dornshuld, E. V., M. Zhang, X. Zhang, T. K. Hollis, and C. E. Webster. Predicting  $^{195}\text{Pt}$  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.
4. Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the  $\text{P}_2$  dimer and the PCCP dimer. *Southeast Theoretical Chemistry Association Annual Meeting (SETCA 2013)*, May 9–11, 2013.
5. Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the  $\text{P}_2$  dimer and the PCCP dimer. *Mississippi Experimental Program to Stimulate Competitive Research State Meeting (EPSCoR)*, April 18, 2013.
6. Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the  $\text{P}_2$  dimer and the PCCP dimer. *53rd Sanibel Symposium*, February 17–22, 2013.
7. Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the  $\text{P}_2$  dimer and the PCCP dimer. *Mississippi Experimental Program to Stimulate Competitive Research Fall Forum (EPSCoR)*, August 28, 2012.
8. Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the  $\text{P}_2$  and PCCP dimers. *Southeast Theoretical Chemistry Association Annual Meeting (SETCA 2012)*, May 17–19, 2012.
9. Dornshuld, E. V. and G. S. Tschumper. Characterization of the potential energy surfaces of the  $\text{P}_2$  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  $\text{P}_2$  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  $\text{P}_2$  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  $\text{P}_2$  and PCCP dimers. *Mississippi Experimental Program to Stimulate Competitive Research State Meeting (EPSCoR)*, April 14, 2011.
13. 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.
2. 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.
3. 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.
4. 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.
5. 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.
6. 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.
7. 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.
8. 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.
9. Adiraju, K., M. Zhang, E. V. Dornshuld, R. W. Lamb, G. Liang, C. E. Webster, and T. K. Hollis. State-of-the-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.
10. 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.
12. 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.
13. 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.
14. 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.
15. 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.

16. 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.
17. Zhang, M., E. V. Dornshuld, X. Zhang, and C. E. Webster. Predicting metal complex reactivity for energy applications: Donicity of meridional tridentate ligands:  $^{195}\text{Pt}$  NMR of CCC-NHC Pt pincer square planar complexes. *Feeding and Powering the World 2016: Building the Network*, University, MS, July 25–26, 2016.
18. 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.