Virginia Tech Graduate Research Assistant Crawford Group Phone: +1 (901) 240-0487 Department of Chemistry (0212) Davidson Hall Rm 420 1040 Drillfield Drive Blacksburg, Virginia 24061

Education

Virginia Tech

Ph.D. Candidate, Chemistry, (expected) 2021. Current GPA: 3.77

Advisor: Prof. T. Daniel Crawford

Mississippi College

B.S., Summa Cum Laude, Chemical Physics, 2016. GPA: 3.90

Advisor: Prof. David H. Magers

Thesis: "The Conventional Strain Energies of Cyclobutadiene and its Dimethyl- and

Dinitro- Derivatives"

Southwest Tennessee Community College

Transfer credit, Chemistry, 2014. Advisor: Dr. Daniel Osborne

Professional Workshops and Summer Schools

2019 European Summer School in Quantum Chemistry, Palermo, Italy

2017 MolSSI Software Summer School, Virginia Tech

2017 Molecular Response Properties Summer School, Virginia Tech

2016 ACS COMP Undergraduate Research Workshop, San Diego, California

Research

Publications

- 1. "Machine-Learning Coupled Cluster Properties through a Density Tensor Representation," B. G. Peyton, C. Briggs, R. D'Cunha, J. T. Margraf, and T. D. Crawford, *J. Phys. Chem. A* 124, 4861-4871 (2020).
- 2. "Basis Set Superposition Errors in the Many-Body Expansion of Molecular Properties," B. G. Peyton and T. D. Crawford, *J. Phys. Chem. A* **123** (20), 4500-4511 (2019).

Code Contributions

Psi4: Open-Source Quantum Chemistry (github.com/psi4/psi4) Psi4Education (github.com/psi4education/psi4education)

Presentations

Talk Georgia Tech Machine Learning in Chem. Seminar Series 2020, Virtual

Poster Fall ACS 2020, Virtual

Talk/Poster VCTC 2020, Virtual

Talk, PsiCon 2019, Atlanta, Georgia

Poster, ESQC 2019, Palermo, Italy

Poster, SETCA 2019, Knoxville, TN

Talk, PsiCon 2017, Blacksburg, Virginia

Poster, MS ACS Honors Banquet 2016, 1st prize, Starkville, MS

Talk, MCTC Resarch Symposium, 2016, 1st prize, Tougaloo, MS

Poster, Spring ACS 2016, San Diego, California

Talk, SURC 2016, 2nd prize, Atlanta, Georgia

Poster, CCTCC 2015, Jackson, MS

Poster, SWRM/SERMACS 2015, Memphis, TN

Talk, MCTC Research Symposium 2015, Clinton, MS

Poster, MS ACS Honors Banquet 2015, 2nd prize, Hattiesburg, MS

Poster, SURC 2015, Tuscaloosa, AL

Poster, SWRMACS 2015, Fort Worth, TX

Awards

Graduate School Doctoral Assistantship Award @ Virginia Tech Spring '21

Joseph Barnhill Memorial Award in Chemistry @ Mississippi College '16

Alpha Chi Honor Society @ Mississippi College '16

Who's Who Among Students in American Universities and Colleges? '15

Dean's List @ Mississippi College '16

President's List @ Mississippi College '14/'15

Trustee Scholar @ Mississippi College '14-'16

Dean's List @ Southwest Tennessee Community College '13/'14

Phi Theta Kappa Honor Society '13

Teaching

Virginia Tech

Physical Chemistry I Lab

Teaching assistant, wet labs, prelab lectures

Development of prelab quiz software

General Chemistry I Lab

Teaching assistant, wet labs

Mississippi College

Physical Chemistry I Lab

Teaching assistant, wet labs, Mathcad exercises

General Chemistry I Lab

Teaching assistant, wet labs

Southwest Tennessee Community College

Organic Chemistry I Lab

Teaching assistant, wet labs