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CURRICULUM VITAE

INTERESTS

- Catalysis; Separations; Reaction Engineering; Quantum Computing; Physical Chemistry; Computational Catalysis; CO_2 Utilization, Methane Conversion, Clean Energy; Zeolites; Lightweight Materials, Integrated Computational and Materials Engineering

EDUCATION

- **Ph.D. Chemical Engineering** [August 2016]
  University of South Carolina (USC)-Columbia, SC
  Thesis Title: Uncertainty Quantification in Computational Catalysis
- **M.S. Chemical Engineering** [December 2013]
  University of South Carolina (USC)-Columbia, SC
  Thesis Title: Comparison of a Particle Filter and Other State Estimation Methods for
- **B.S. Chemical & Biomolecular Engineering** [December 2009]
  Georgia Institute of Technology-Atlanta, GA

PROFESSIONAL EXPERIENCE

- **Senior Engineer, Modelling and Simulation** [August 2023-]
  American Lightweight Materials Manufacturing Innovation Institute (LIFT)
- **Research Scientist** [September 2022-July 2023]
  Department of Mechanical and Aerospace Engineering
- **Data Scientist** [January 2022-August 2022]
  Flexible time, Digital Americas, Linde, plc, Tonawanda, NY
- **Adjunct Appointment Chemical and Biological Engineering** [January 2020-present]
  University at Buffalo, the State University of New York
- **Assistant Professor of Research Data Science** [January 2019-December 2021]
  University at Buffalo, the State University of New York
- **Postdoctoral Fellow** [September 2016-December 2018]
  University of Michigan-Ann Arbor, Department of Chemistry

SELECTED JOURNAL PUBLICATIONS

1. Bello, R.; Kyriakidou, E. A.; **Walker, Eric A.** Dataset for CO_2 purification via a zeolite material. *Results Surf. Interfaces* **2024**, *17*, 100177.

2. Canavan, J.; Giewont, K.; Kyriakidou**,** E. A.; **Walker, E. A.** Feasibility of Methane Oxidation on SSZ-13 Bridged Pd_2O_x Sites: A Theoretical Study. *J. Phys. Chem. C,* **2022**, *126*, 17123-17134.

3. Becerra, A. J.; Diaz-Ibarra, O. H.; Kim, K.; Debusschere, B.; **Walker, E. A.** How a Quantum Computer Could Accurately Solve a Hydrogen-Air Combustion Model. *Digital Discovery,* **2022**, *1*, 511-518.

4. **Walker, E. A.** Bayesian Statistics in Catalysis: A Perspective. *Curr. Opin. Chem. Eng.* **2022**, *36*, 100820.

5. Lee, J.; Giewont, K.; Chen, J.; Liu, C.-H.; **Walker, E. A.**; Kyriakidou, E. A. Ag/ZSM-5 Traps for C_2H_4 and C_7H_8 Adsorption under Cold-Start Conditions. *Micropor. Mesopor. Mat.,* **2021**, *327,* 111428.

6. Becerra, Alejandro; Prabhu, Anand; Rongali, Mary Sharmila; Velpur, Sri Charan Simha; Debusschere, Bert; **Walker, Eric A.**, How a Quantum Computer Could Quantify Uncertainty in Microkinetic Models. *J. Phys. Chem. Lett.* **2021**, *12*, 6955-6960.

7. Giewont, K.; Kyriakidou, E. A.; **Walker, E. A.** Investigation of Potential Catalytic Active Sites of Pd/SSZ-13: A DFT Perspective. *J. Phys. Chem. C*, **2021**, *125* (28), 15262–15274.

8. **Walker, E. A.**; Ravisankar, K.; Savara, A. CheKiPEUQ Intro 2: Harnessing Uncertainties from Data Sets, Bayesian Design of Experiments in Chemical Kinetics. *ChemCatChem*, **2020**, *12* (21), 5401-5410. Special Collection: Data Science in Catalysis.

9. Horvatits, C.; Lee, J.; Kyriakidou, E. A.; **Walker, E. A.** Characterizing Adsorption Sites on Ag/SSZ-13 Zeolites: Experimental Observations and Bayesian Inference. *J. Phys. Chem. C*, **2020**, 124 (35), 19174-19186. Special Issue: Machine Learning in Physical Chemistry.

10. Horvatits, C.; Li, D.; Dupuis, M.; Kyriakidou, E. A.; **Walker, E. A.** Ethylene and Water Co-Adsorption on Ag/SSZ-13 Zeolites: A Theoretical Study. *J. Phys. Chem. C.*, **2020**, 124 (13), 7295-7306.

SERVICE

1. Session Chair, New Developments in Computational Catalysis American Institute of Chemical Engineers Annual Meeting
2. Reviewer, ACS Catalysis, Journal of Catalysis, and others