Venkata Swaroopa Datta, DEVULAPALLI (Ph.D.)

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Webpage **LinkedIn**

Technical Expertise

Scientific

- Ultra-High vacuum coupled Infrared spectroscopy and Mass spectrometry
- Gas adsorption studies
- UV-vis, NMR, FTIR and Raman spectroscopy
- Scanning tunneling microscopy (STM)
- X-ray diffraction spectroscopy (at Argonne National Lab, BM-17)
- Basics of materials synthesis

Computer Based

- ChemDraw
- IGOR pro
- MS office
- LabVIEW
- OPUS
- Gwyddion

Education

2017 Fall – 2023 Spring| Ph.D.| Department of Chemistry| Temple University

Ph.D. thesis: *"The Chemistry of Metal Oxyhydroxides and their 3D Porous Materials for the Capture, Transport and Degradation of Toxic Chemicals"*

Current GPA: 3.96

Mentor: Dr. Eric Borguet

2013-2018| B.Sc. - M.Sc.| Indian Institute of Science Education and Research (IISER, Pune, India) | Major: Chemistry

Master's thesis: "*Temperature Programmed Infrared and Mass Spectrometry Analysis of Interactions of Covalent Organic Frameworks with Simple Polar and Nonpolar Organic Molecules*"

Mentors: Dr. Eric Borguet (Temple University), Dr. Ramanathan Vaidhyanathan (IISER, Pune)

Research Experience

2017-Present | Graduate Research Assistant (Mentor: Dr. Eric Borguet, Temple University, Philadelphia, USA)

In situ IR spectroscopy to detect and characterize missing linker defects in UiO-67 MOFs. (One paper published, one in preparation)

Discoveries

- Spectroscopic identification of water-capped, missing linker defect sites (active species aiding catalysis) in UiO-67.
- First report of IR spectroscopic evidence of novel NH-π interactions, revealing unconventional binding sites for NH_3 adsorbed in UiO-67 MOFs and potential binding sites for other toxic gases.

Thermal properties of UiO-67 MOFs and impact of guests. (One paper published, one in preparation)

Discoveries

- *In situ* IR and X ray studies reveal distortion of COO^- groups (present on linkers) occurring during heating causing the buckling of linkers and negative thermal expansion (NTE).
- Water uptake in MOFs switches from NTE to positive thermal expansion (PTE).

Impact of the Lewis acidity of Zr and Hf oxyhydroxides and their MOFs on catalytic hydrolysis. (One paper published, one submitted)

Discoveries

- Hydrolysis of CWA simulant (DMNP) is proportional to Lewis acidity of the metal.
- Correlation in catalytic activities of MOFs and precursors: Efficiency of Precursor A > Precursor B => Efficiency of MOF A > MOF B; Paradigm for judicious choice of metal for synthesizing MOFs for applications in hydrolysis.

Development and characterization of catalytic and photocatalytic nanoparticle decorated COF hybrids. (One paper published)

Discoveries

Discovered a one pot synthesis protocol which uses simple, benign chemicals to obtain robust nanoparticle-COF hybrids, which display excellent catalytic properties compared to reported materials.

Writing of successful proposals for synchrotron X-ray experiments at Argonne National Lab.

2013-2018 | Undergraduate Student Researcher (IISER, Pune, India)

- Materials synthesis for photocatalytic water splitting (supervisor: Dr. R. Vaidhyanathan).
- Au/Ag catalyzed glycosylation of partially protected sugars (supervisor: Dr. S. Hotha).

Publications

1. Interplay between Intrinsic Thermal Stability and Expansion Properties of Functionalized UiO-67 Metal–Organic Frameworks, Goodenough, I.; Devulapalli, V. S. D.; Xu, W.; Boyanich, M. C.; Luo, T.-Y.; De Souza, M.; Richard, M.; Rosi, N. L.; Borguet, E., *Chemistry of Materials,* 2020, 33 (3), 910-920. DOI: 10.1021/acs.chemmater.0c03889. *Selected as Journal Front Cover.*
2. Tuning the Lewis acidity of Metal–Organic Frameworks for Enhanced Catalysis, Devulapalli, V. S. D.; Richard, M.; Luo, T.-Y.; De Souza, M. L.; Rosi, N. L.; Borguet, E., *Dalton Transactions,* 2021, 50 (9), 3116-3120. DOI: 10.1039/D1DT00180A. *Selected as Journal Front Cover.*
3. Identifying UiO-67 Metal-Organic Framework Defects and Binding Sites through Ammonia Adsorption, Devulapalli, V. S. D.; McDonnell, R. P.; Ruffley, J. P.; Shukla. P. B.; Luo, T. Y.; De

Souza, M. L.; Das, P.; Rosi, N. L.; Johnson, J. K.; Borguet, E., *ChemSusChem*, 2022, 15 (1), e202102217. DOI: 10.1002/cssc.202102217.

4. Synergistic Electronic Effects in Au Co Nanoparticles Stabilized in Triazine Covalent Organic Framework Catalyst, Devulapalli, V. S. D.; Kushwaha, R.; Ovalle, E.; Singh, H. D.; Shekhar, P.; Chakraborty, D.; Vinod, C.P.; Vaidhyanathan, R.; Borguet, E., *ACS Applied Nano Materials,* **2022**, 5 (4), 4744-4753. DOI: 10.1021/acsanm.1c04212.
5. Anomalous Infrared Intensity Behavior of Acetonitrile Diffused into UiO-67, McDonnell, R.; Devulapalli, V. S. D.; Choi, T. H.; McDonnell, L.; Das, P.; Rosi, N. L.; Johnson, J. K.; Borguet, E., Submitted to *Chemistry of Materials,* **2023**.
6. COF Supported Zirconium Oxyhydroxide as a Versatile Heterogeneous Catalyst for Knoevenagel Condensation and Nerve Agent Hydrolysis, Shekhar, P.#; Devulapalli, V. S. D.#; Reji R.; Singh, H. D.; Tokarz, J.; Mahle, J. J.; Jose, A.; Torris, A.; Peterson, G. W.; Borguet, E., Vaidhyanathan, R., Anticipated submission: Submitted to *Chemistry of Materials,* **2023**.
7. Impact of pH on Lewis Acidic Metal Oxyhydroxide Formation and Hydrolysis of Organophosphorus Nerve Agent Simulant, Devulapalli, V. S. D.; Nero, T. R.; Sahraoui, I.; Borguet, E., Anticipated submission: August **2023.**
8. Isabella Goodenough, Boyanich, M. C.; Castellana, L.; Devulapalli, V. S. D.; Xu, W.; Luo, T.-Y.; De Souza, M.; Richard, M.; Rosi, N. L.; Borguet, E., The Vibrational Signature of Metal-Organic Frameworks Interactions with Polar and Non-polar Solvents. Anticipated submission: August **2023**.

Oral-Presentations

1. "*Tuning the Lewis acidity of metal–organic frameworks for enhanced catalysis*" Catalytic and Photocatalytic Degradation of Pollutants and Chemical Threat Agents: New Materials and in Operando Methods; Division of Catalysis Science & Technology; Spring ACS National Meeting, Spring, April 2021, (Virtual).
2. "*Catalytic Degradation of Organic Pollutants Using Hybrid Covalent Organic Frameworks*" Catalytic and Photocatalytic Degradation of Pollutants and Chemical Threat Agents: New Materials and in Operando Methods; Division of Catalysis Science & Technology; Spring ACS National Meeting, Spring, April 2021, (Virtual).
3. *"Simple Analytical Tools to Understand and Evaluate the Impact of Lewis Acidity on the Catalytic Activity of Metal Oxyhydroxides"* Fall Eastern Analytical Symposium, November 2021, Crowne Plaza Princeton-Conference Center, Plainsboro, NJ, USA.
4. *"Understanding Binding sites and Defects in UiO-67 Metal-Organic Frameworks: An in-situ Infrared Spectroscopic Study*" Summer ACS-Middle Atlantic Regional Meeting, June 2022, New Jersey Institute of Technology, Trenton, NJ, USA.

Poster-Presentations

1. Venkata Swaroopa Datta, Isabella Goodenough, Mikaela Boyanich, Tian-Yi Luo, Nathaniel L. Rosi, Eric Borguet. "*Thermal stability of zirconium MOFs and their interactions with ammonia: A temperature programmed in-situ IR study"*. Thermal Analysis Forum of Delaware Valley, December 2018, University of Pennsylvania, Philadelphia, PA, USA.
2. Venkata Swaroopa Datta, Isabella Goodenough, Melissandre Richard, Debanjan Chakraborty, Dinesh Mullangi, Ramanathan Vaidhyanathan, Eric Borguet. "*A thermal study of interactions*

between covalently bonded organic frameworks and industrially important analytes". Thermal Analysis Forum of Delaware Valley, April 2018, Rutgers University, Camden, NJ, USA.

3. Venkata Swaroopa Datta, Isabella Goodenough, Melissandre Richard, Debanjan Chakraborty, Dinesh Mullangi, Ramanathan Vaidhyanathan, Eric Borguet. "*Interactions of Simple Organic Molecules with Covalent Organic Frameworks*". The Younger Chemists Committee Philadelphia Section, April 2018, Temple University, Philadelphia, PA, USA.
4. Venkata Swaroop Datta Devulapalli, Edwin Ovalle, Debanjan Chakraborty, Ramanathan Vaidhyanathan, Eric Borguet. "*Catalytic Degradation of Methyl Orange by Robust Nanoparticle-Covalent Organic Framework (NP-COF) Hybrid"*. Philadelphia Inorganic Colloquium, Spring 2018, Philadelphia, PA, USA.
5. Venkata Swaroopa Datta Devulapalli; Melissandre Richard; Tian-Yi Luo; Nathaniel. L Rosi; Eric Borguet, *Hydrolysis of nerve agent simulant DMNP by zirconium MOFs – "Identification of active species".* Gordon Research Seminar: Nanoporous Materials and their Applications, August 2019, Andover, NH, USA.
6. Venkata Swaroopa Datta Devulapalli, Ryan McDonnell, Isabella Goodenough, Tian-Yi Luo, Nathaniel L. Rosi, Eric Borguet, *Interactions between ammonia and UiO-67 zirconium MOFs.* Gordon Research Conference: Nanoporous Materials and their Applications, August 2019, Andover, NH, USA.

Awards

2015:	Summer Research Fellowship, Indian Institute of Science Education and Research Pune, Ministry of Human Resource and Development, Government of India.
2013-18:	Innovation in Science Pursuit for Inspired Research (INSPIRE) fellowship, Department of Science and Technology, Government of India.
May 2017:	First student selected for IISER-TU Dual Masters Doctoral Degree (DMDD).
August 2021:	2nd place for oral presentation as ACS Eastern US, Younger Chemists Committee (YCC) virtual research symposium and chemistry career expo.
December 2021:	Daniel Swern Fellowship for Outstanding Research.
June 2022:	Summer Research Support.
December 2022:	Francis Case Fellowship for Outstanding Creativity and Productivity in Research.

Teaching Experience at Temple University

2017 (Fall):	TA for General Chemistry (I) Laboratory course
2017 (Fall):	TA for "Chemistry for Engineers"
2018 (Spring):	TA for General Chemistry (I) Laboratory course
2018 (Fall):	TA for "Chemistry for Engineers"
2019 (Spring):	TA for General Chemistry (I) Laboratory course
2020 (Fall):	½ TA for "Chemistry for Engineers"
2021 (Spring):	½ TA for Physical Chemistry-I

Leadership Roles

2017- Present:	Graduate research mentor (Borguet group), Mentored (11) undergraduate students, Graduate student (2) and trained them to perform experiments, data analysis/interpretation.
2018:	Organizing team member for Younger Chemists Committee (YCC) conference at Temple University.
2018:	Co-organized "Kurt J. Lesker University" workshop at Temple University.
2020-22:	Member of Council on Student Involvement (CSI), Chemistry Department, Temple University.
Summer 2021:	Mentor and train high school student in basic chemistry/research under Temple Science Preparatory Research Opportunities for Underrepresented Teens (SPROUT) program.
2021- present:	Catalysis and Porous Materials team leader (Borguet group).

References

1. Dr. Eric Borguet (Research advisor)
   Hazel Tomlinson Professor of Chemistry
   Temple University
   eborguet@temple.edu

2. Dr. Wenqian Xu (Collaborator)
   Beamline Scientist
   Argonne National Lab
   wenqianxu@anl.gov