

David C. Cantu

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<https://www.unr.edu/cme/people/cantu>**Positions**

<u>Assistant Professor</u> , University of Nevada, Reno	2017 – Present
<u>Scientist</u> , Pacific Northwest National Laboratory	2017 – 2017
<u>Post Doctorate Research Associate</u> , Pacific Northwest National Laboratory	2013 – 2017

EducationPh.D. Chemical Engineering, Iowa State University, 2013B.S. Chemical Engineering, Tecnologico de Monterrey (ITESM), Mexico, 2008**Awards**

New Doctoral Investigator Award, American Chemical Society Petroleum Research Fund, 2019

Outstanding Performance Award, Pacific Northwest National Laboratory, 2014

Graduate Research Excellence Award, Graduate College, Iowa State University, 2013

Publications (*H-index=15, 988 citations, as of 02/2021 in Google Scholar*)

36. Cantu DC, “Predicting lanthanide coordination structures with molecular simulation”, in Volume 651: Rare-Earth Element Biochemistry: Characterization and Applications of Lanthanide-Binding Biomolecules”, *Methods in Enzymology*, **2021**, *In Press*.
35. Kaliakin DS, Sobrinho J, Monteiro JHSK, de Bettencourt-Dias A, Cantu DC, “Solution structure of a europium-nicotianamine complex supports that phytosiderophores bind lanthanides”, *Physical Chemistry Chemical Physics*, **2021**, DOI: 10.1039/d0cp06150f
34. Shiery RC, Fulton JL, Balasubramanian M, Nguyen MT, Lu JB, Li J, Rousseau R, Glezakou VA, Cantu DC, “Coordination sphere of lanthanide aqua ions resolved with ab initio molecular dynamics and X-ray absorption spectroscopy”, *Inorganic Chemistry*, **2021**, DOI: 10.1021/acs.inorgchem.0c03438
33. Mott TC, Kivstik PM, Panorska AK, Cantu DC. “Comparing conditional probabilities and statistical independence in layers of protection analysis”, *Process Safety Progress*, **2020**, e12215.
32. Kollias L, Cantu DC, Glezakou VA, Rousseau R, Salvalaglio M. “On the role of enthalpic and entropic contributions to the conformational free energy landscape of MIL-101(Cr) secondary building units”, *Advanced Theory and Simulations*, **2020**, 3, 2000092.
31. Bañuelos JL, Lee MS, Nguyen MT, Zhang D, Malhotra D, Cantu DC, Glezakou VA, Rousseau R, Headen TF, Dalglish RM, Heldebrant DJ, Graham TR, Han KS, Saunders SR. “Subtle changes in hydrogen bond orientation result in glassification of carbon capture solvents”, *Physical Chemistry Chemical Physics*, **2020**, 22, 19009-19021.
30. Cantu DC, Malhotra D, Nguyen MT, Koech PK, Zhang D, Glezakou VA, Rousseau R, Page J, Zheng R, Perry RJ, Heldebrant DJ. “Molecular-level overhaul of gamma-aminopropyl aminosilicone/triethylene glycol post-combustion CO₂-capture solvents”, *ChemSusChem*, **2020**, 13,

3429-3438.

29. Nguyen MT, Akhade SA, Cantu DC, Lee MS, Glezakou VA, Rousseau R. “Electro-reduction of organics on metal cathodes: A multiscale-modeling study of benzaldehyde on Au (111)”, *Catalysis Today*, **2020**, 350, 39-46.
28. Lu J, Cantu DC, Nguyen MT, Li J, Glezakou VA, Rousseau R. “Norm-conserving pseudopotentials and basis sets optimized for lanthanide molecules and solid-state compounds”, *Journal of Chemical Theory and Computation*, **2019**, 15, 5987-5997.
27. Kollias L, Cantu DC, Tubbs MA, Rousseau R, Glezakou VA, Salvalaglio M. “Molecular level understanding of the free energy landscape in early stages of metal–organic framework nucleation”, *Journal of the American Chemical Society*, **2019**, 141, 6073-608.
26. Malhotra D, Cantu DC, Koech PK, Heldebrant DJ, Karkamkar A, Zheng F, Bearden MD, Rousseau R, Glezakou VA. “Directed hydrogen bond placement: low viscosity amine solvents for CO₂ capture”, *ACS Sustainable Chemistry & Engineering*, **2019**, 7, 7535-7542.
25. Singh N, Nguyen MT, Cantu DC, Mehdi B, Browning ND, Fulton JL, Zheng J, Balasubramanian M, Gutierrez OY, Glezakou VA, Rousseau R, Govind N, Camaioni D, Campbell CT, Lercher JA. “Carbon-supported Pt during aqueous phenol hydrogenation with and without applied electrical potential: X-ray absorption and theoretical studies of structure and adsorbates”, *Journal of Catalysis*, **2018**, 368, 8-19.
24. Cantu DC, Padmaperuma AB, Nguyen MT, Akhade SA, Yoon Y, Wang YG, Lee MS, Glezakou VA, Rousseau R, Lilga MA. “A combined experimental and theoretical study on the activity and selectivity of the electrocatalytic hydrogenation of aldehydes”, *ACS Catalysis*, **2018**, 8, 7645-7658.
23. Nguyen MT, Mu R, Cantu DC, Lyubinetsky I, Glezakou VA, Dohnalek Z, Rousseau R. “Dynamics, stability, and adsorption states of water on oxidized RuO₂(110)”, **2017**, *The Journal of Physical Chemistry C*, 121, 18505-18515.
22. Cantu DC, Wang YG, Yoon Y, Glezakou VA, Rousseau R, Weber RS. “Heterogeneous catalysis in complex, condensed reaction media”, **2017**, *Catalysis Today*, 289, 231-236.
21. Heldebrant DJ, Koech PK, Rousseau R, Glezakou VA, Cantu DC, Malhotra D, Zheng F, Whyatt G, Freeman CJ, Bearden MD. “Are water-lean solvent systems viable for post-combustion CO₂ capture?”, **2017**, *Energy Procedia*, 114, 756-763.
20. Cantu DC, Malhotra D, Koech PK, Heldebrant DJ, Zheng F, Freeman CJ, Rousseau R, Glezakou VA. “Integrated solvent design for CO₂ capture and viscosity tuning”, **2017**, *Energy Procedia*, 114, 726-734.
19. Heldebrant DJ, Koech PK, Glezakou VA, Rousseau R, Malhotra D, Cantu DC. “Water-lean solvents for post-combustion CO₂ capture: fundamentals, uncertainties, opportunities, and outlook”, **2017**, *Chemical Reviews*, 117, 9594-9624.
18. Malhotra D, Koech PK, Heldebrant DJ, Cantu DC, Zheng F, Glezakou VA, Rousseau R. “Reinventing design principles for developing low-viscosity carbon dioxide-binding organic liquids for flue gas clean up”, **2017**, *ChemSusChem*, 10, 636-642.
17. Xu CQ, Lee MS, Wang YG, Cantu DC, Li J, Glezakou VA, Rousseau R. “Structural rearrangement of Au-Pd nanoparticles under reaction conditions: an ab-initio molecular dynamics study”, **2017**, *ACS Nano*, 11, 1649-1658.
16. Cantu DC, Malhotra D, Koech PK, Heldebrant DJ, Zheng F, Freeman CJ, Rousseau R, Glezakou VA. “Structure-property reduced order model for viscosity prediction in single-component CO₂-binding organic liquids”, **2016**, *Green Chemistry*, 18, 6004-6011. [In journal cover, 11/21/2016]
15. Wang YG, Cantu DC, Lee MS, Li J, Glezakou VA, Rousseau R. “CO oxidation on Au/TiO₂: condition dependent active sites and mechanistic pathways”, **2016**, *Journal of the American Chemical Society*, 138, 1234-1242.

Society, 138, 10467-10476.

14. Cantu DC, Lee J, Lee MS, Heldebrant DJ, Koech PK, Freeman CJ, Rousseau R, Glezakou VA. "Dynamic acid/base equilibrium in single component switchable ionic liquids and consequences of viscosity", **2016**, *The Journal of Physical Chemistry Letters*, 7, 1646-1652.
13. Mu R, Cantu DC, Glezakou VA, Lyubinetsky I, Rousseau R, Dohnalek Z. "Deprotonated water dimers: the building blocks of segmented water chains on rutile RuO₂(110)", **2015**, *The Journal of Physical Chemistry C*, 119, 23552-23558. [In journal cover, 10/15/2015]
12. Heldebrant DJ, Glezakou VA, Koech PK, Mathias P, Cantu DC, Rousseau R, Malhotra D, Bhakta M, Bearden MD, Freeman CJ, Zheng F. "Evaluating transformational solvent systems for post-combustion CO₂ separations", **2014**, *Energy Procedia*, 63, 8144-8152.
11. Cantu DC, McGrail BP, Glezakou VA. "Formation mechanism of the secondary building unit in a chromium terephthalate metal-organic framework", **2014**, *Chemistry of Materials*, 26, 6401-6409. [In journal cover, 11/25/2014]
10. Mu R, Cantu DC, Lin X, Glezakou VA, Wang Z, Lyubinetsky I, Rousseau R, Dohnalek Z. "Dimerization induced deprotonation of water on RuO₂(110)", **2014**, *The Journal of Physical Chemistry Letters*, 5, 3445-3450.
9. Cantu DC, Ardevol A, Rovira C, Reilly PJ. "Molecular mechanism of a hotdog-fold acyl-CoA thioesterase", **2014**, *Chemistry A European Journal*, 20, 9045-9051.
8. Cantu DC, Dai T, Beversdorf ZS, Reilly PJ. "Structural classification and properties of ketoacyl reductases, hydroxyacyl dehydratases, and enoyl reductases", **2012**, *Protein Engineering Design & Selection*, 25, 803-811.
7. Chen Y, Elizondo-Noriega A, Cantu DC, Reilly PJ. "Structural classification of biotin carboxyl carrier proteins", **2012**, *Biotechnology Letters*, 34, 1869-1875.
6. Cantu DC, Forrester MJ, Charov K, Reilly PJ. "Acyl carrier protein structural classification and normal mode analysis", **2012**, *Protein Science*, 21, 655-666.
5. Jing F, Cantu DC, Tvaruzkova J, Chipman JP, Nikolau BJ, Yandeau-Nelson MD, Reilly PJ. "Phylogenetic and experimental characterization of an acyl-ACP thioesterase family reveals significant diversity in enzymatic specificity and activity", **2011**, *BMC Biochemistry*, 12, 44.
4. Chen Y, Kelly EE, Masluk RP, Nelson CL, Cantu DC, Reilly PJ. "Structural classification and properties of ketoacyl synthases", **2011**, *Protein Science*, 20, 1659-1667.
3. Cantu DC, Chen Y, Lemons ML, Reilly PJ. "ThYme: a database for thioester-active enzymes", **2011**, *Nucleic Acids Research*, 39, D342-D346.
2. Cantu DC, Chen Y, Reilly PJ. "Thioesterases: A new perspective based on their primary and tertiary structures", **2010**, *Protein Science*, 19, 1281-1295.
1. Cantu DC, Nerinckx W, Reilly PJ. "Theory and computation show that Asp463 is the catalytic proton donor in human endoplasmic reticulum α -(1 \rightarrow 2)-mannosidase I", **2008**, *Carbohydrate Research*, 343, 2235-2242.

Patents

U.S. Patent Application: "Novel diamine solvent system for CO₂ capture"

U.S. Patent 10,773,205: "Capture and release of acid gasses using tunable organic solvents with aminopyridine"

U.S. Patent 10,722,837: "Capture and release of acid gasses using tunable organic solvents with aminopyridine"

U.S. Patent 10,456,739: "Capture and release of acid gasses using tunable organic solvents with binding

organic liquids”

U.S. Patent 10,434,460: “Capture and release of acid gasses using tunable organic solvents with aminopyridine”

U.S. Patent 10,130,907: “Capture and release of acid gasses using tunable organic solvents with aminopyridine”

Funding

National Science Foundation, “Elements: The ThYme database and identifying representative amino acid sequences that originate thioester-active enzyme families”, 2020 – 2023

American Chemical Society Petroleum Research Fund, “Uncovering the Role of Lanthanum in Faujasite Hydrothermal Stability”, 2019 – 2021

Research Mentoring at the University of Nevada, Reno

Postdoctoral or Research Associates

Caio Carvalho: 2020 – Current

Danil Kaliakin: 2020 – 2020

Graduate Students

Benjamin Caswell: 2020 – Current

Richard Shiery: 2018 – Current

Timothy Mott: M.S. 2020

Undergraduate Students

Stuart McElhany: 2019 – Current

Kyle Cooper: 2018 – 2020

Robin Dietrich: 2018 – 2020

Coleton Meyer: 2017 – 2019

Aayushman Mishra: 2018

Shane Johnson: 2018

Desi Imbiri: 2017 – 2018

Michelle Nguyen: 2017 – 2018

Ethan Skemp: 2017 – 2018

Courses taught at the University of Nevada, Reno

CHE 245, *Computer Applications in Chemical Engineering*, Spring 2018, Fall 2019, Fall 2020

CHE 451, *Process Control*, Spring 2020, Spring 2021

CHE 485, *Separation Processes*, Fall 2017, Fall 2018, Fall 2019, Fall 2020

Presentations (Invited Talk)**

“Predicting the structure of lanthanide-ligand complexes in solution with ab initio molecular dynamics”, *American Institute of Chemical Engineering Annual Meeting*, Virtual, 2020.

“Predicting lanthanide-ligand complex structures in the condensed phase with ab initio molecular dynamics”, *2020 Chemical Separations Gordon Research Conference*, Galveston, TX, 2020.

“Simulating lanthanide-ligand complexes in the condensed phase with ab initio molecular dynamics”, *CPMD2019*, Lausanne, Switzerland, 2019.

- ** “Modeling specificity in adsorption and charge transfer on solid/liquid interfaces”, *Northwest Regional Meeting of the American Chemical Society*, Richland, WA, 2018
- ** “Speciation at Solid/Liquid Interfaces in the Thermal or Electrochemical Hydrogenation of Organic Compounds”, *Institute for Integrated Catalysis Advisory Board Meeting*, Richland, WA, 2017.
- ** “Molecular Design Strategies to Reduce the Viscosity of CO₂ Capture Solvents”, *Chemical and Biological Engineering Department, Montana State University*, Bozeman, MT, 2016.
- ** “Molecular Design Strategies to Reduce the Viscosity of CO₂ Capture Solvents”, *Chemical and Materials Engineering Department, University of Nevada, Reno*, Reno, NV, 2016.
- “Computational Modeling of Electrochemical Bio-Oil Upgrading”, *American Institute of Chemical Engineering Annual Meeting*, San Francisco, CA, 2016.
- “Molecular Design of Carbon Capture Solvents”, *American Institute of Chemical Engineering Annual Meeting*, San Francisco, CA, 2016.
- ** “Molecular Design Strategies to Reduce the Viscosity of CO₂ Capture Solvents”, *Pacific Northwest National Laboratory*, Richland, WA, 2016.
- ** “Molecular Design of Carbon Capture Solvents”, *Department of Chemical and Biological Engineering, Iowa State University*, Ames, IA, 2016.
- ** “Computational Modeling of Electrochemical BioOil Stabilization” *American Chemical Society National Meeting*, Philadelphia, PA, 2016.
- “Computational Modeling of Electrochemical BioOil Stabilization” *American Chemical Society National Meeting*, San Diego, CA, 2016.
- ** “Molecular Design of Carbon Capture Solvents”, *Department of Chemical Engineering, Auburn University*, Auburn, AL, 2016.
- “Water Dissociation, Diffusion, and Clustering on RuO₂(110)”. *American Institute of Chemical Engineering Annual Meeting*, Salt Lake City, UT, 2015.
- “Molecular Modeling of Non-Aqueous CO₂ Capture Solvents”. *American Institute of Chemical Engineering Annual Meeting*, Salt Lake City, UT, 2015.
- “Uncovering Elementary Reactions in the Formation of a Metal Organic Framework Secondary Building Unit with Density Functional Theory, Simulation and Kinetics”, *FOMMS 2015: Molecular Modeling and the Materials Genome*, Mt. Hood, OR 2015.
- “Molecular Modeling of Non-Aqueous CO₂ Capture Solvents”, *American Chemical Society National Meeting*, Denver, CO, 2015.
- ** “Multi-scale Modeling of Chemical Reactivity in Materials Synthesis”, *Department of Chemical and Biomolecular Engineering, University of Nebraska*, Lincoln, NE, 2015.
- “Formation Mechanism of the Secondary Building Unit in a Chromium Terephthalate Metal Organic Framework”, *Pacific Northwest National Laboratory*, Richland, WA, 2015.
- “Detailed step-by-step reactions towards the synthesis of a MOF”, *American Institute of Chemical Engineering Annual Meeting*, Atlanta, GA, 2014.
- ** “Finding desired enzymes in nature, and understanding enzymatic catalysis”, *Pacific Northwest National Laboratory*, Richland, WA, 2013.
- “Mechanism of a hotdog fold thioesterase-catalyzed reaction proposed by QM/MM metadynamics simulation”, *American Institute of Chemical Engineering Annual Meeting*, Pittsburgh, PA, 2012.
- “Acyl carrier protein classification and normal mode analysis”, *American Institute of Chemical Engineering Annual Meeting*, Pittsburgh, PA, 2012.
- “Phylogenetic and experimental characterization of an acyl-ACP thioesterase family reveals significant

diversity in enzymatic specificity and activity”, *American Institute of Chemical Engineering Annual Meeting*, Minneapolis, MN, 2011.

“ThYme: a database of the primary and tertiary structures of the enzyme and protein groups involved in the synthesis of fatty acids and polyketides”, *Iowa State University–University of Iowa Bioinformatics Meeting*, Ames, IA, 2011.

Professional Affiliations

Sigma Xi, American Institute of Chemical Engineers, American Chemical Society