

DANIEL H. ESS

Professor

Department of Chemistry and Biochemistry

Brigham Young University

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EDUCATION

Ph.D. Comp. Chemistry

University of California, Los Angeles (9/03-10/07)

Advisor: K. N. Houk

B.S. Biochemistry

Brigham Young University, Provo, Utah (2000)

PROFESSIONAL POSITIONS

Professor

Brigham Young University, Provo Utah (9/20-present)

Associate Professor

Brigham Young University, Provo Utah (9/16-9/20)

Assistant Professor

Brigham Young University, Provo Utah (7/10-8/16)

Postdoctoral Scholar

University of North Carolina at Chapel Hill (10/09-6/10)

Comp. Inorganic

Advisors: Cynthia K. Schauer and Thomas J. Meyer

Postdoctoral Scholar

The Scripps Research Institute, Florida (10/07-10/09)

Comp. & Experimental Catalysis

Advisor: Roy A. Periana

California Institute of Technology (10/07-10/09)

Advisor: William A. Goddard, III

OTHER EXPERIENCE

Consultant

Hyconix Inc. (2015-present).

CURRENT FUNDED RESEARCH AREAS

- Computational catalyst design
- Organometallic molecular dynamics
- Computational studies of alkane C-H functionalization reactions
- Computational studies on multinuclear transition-metal catalysis

CURRENT AWARDS

- *National Science Foundation*, “Dynamical Organometallic Mechanisms” CHE-1952420 (PI, 2020-2023)
- *Chevron Phillips Chemical Co.*, “Design of Homogeneous Alpha Olefin Catalysts” (PI, 2014-2021)
- *Phillips 66*, “Computational Optimization of Solid Acid Metal-Organic Frameworks” (PI, 2019-2021)
- *National Science Foundation*, “Theory and Design of Transition-Metal Heterodinuclear and Homodinuclear Catalytic Reactions” CHE-1764194 (PI, 2018-2021)

- *National Science Foundation*, “Chemistry and Biochemistry REU Site to Prepare Students for Graduate School and an Industrial Career” CHE-1757627 (PI, 2018-2021) \$331,950; renewal (PI, 2021-2024) CHE-2050872
- *U.S. Department of Energy, Office of Basic Energy Sciences, Catalysis Sciences*, “Theory of Main-Group, p-Block Hydrocarbon Functionalization Reactions” (PI, 2017-2020) and renewal “Modeling and Design of Main-Group Metal Catalyzed Alkane C-H Functionalization Reactions” (PI, 2020-2023) DE-SC0018329
- *National Institutes of Health, NIGMS*, “Asymmetric N-H/N-alkyl olefin aziridinations and ring-opening transformations” 1R35GM136373- 01 (subcontract, 2020-2025)

COMPLETED AWARDS

- *National Institutes of Health, NIGMS*, “Asymmetric N-H/N-alkyl olefin aziridinations and ring-opening transformations” 1R01GM114609-01 (subcontract, 2015-2019)
- *State of Utah, Principle Energy Issues Program, Utah Research Triangle*, “Catalytic Conversion of Carbon Dioxide to Carbon Monoxide and Methanol” (PI, 2014-2015)
- *U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences*, “Energy Frontier Research Center, Center for Catalytic Hydrocarbon Functionalization” DE-SC0001298 (subcontract, Co-PI, 2010-2014)
- *American Chemical Society Petroleum Research Foundation*, “Quantum Mechanical Investigation of Fundamental Concepts in Hydrocarbon C-H Bond Activation” (PRF #51081-DNI3) (PI, 2011-2014)

SOFTWARE DEVELOPMENT

<https://github.com/DanielEss-lab>

- Milo: a quasiclassical direct dynamics program (Python).
- MECPro: Efficient Python program to locate minimum energy crossing points for organometallic reactions.
- Taylor: A program to automate transition state searching.
- Mason: A program to automate transition state building.

CHEMISTRY CAMPS

- Creator and co-director of BYU Chem Camp for children ages 9-12 (<https://chemcamp.byu.edu/9-12>) >300 children from 2016-present.
- Creator and co-director of BYU BioChem Camp for youth ages 13-14. (<https://chemcamp.byu.edu/13-14>) >100 youth from 2017-present.

SUMMER VISITING UNDERGRADUATE RESEARCH PROGRAM

<https://reu.chem.byu.edu/>

- PI and director of the NSF-funded Chemistry and Biochemistry Research Experiences for Undergraduates REU program “*Chemistry and Biochemistry REU Site to Prepare Students for Graduate School and an Industrial Career*”. Established 2018, the goal of this program is to provide a pathway to graduate school. This site hosts 10 visiting undergraduate students each year and 2 high school teachers (RET).

COURSES TAUGHT

- Organic chemistry 1 and 2: Chem 351, 351M, 352, 352M, and 357. These are large section classes ranging from 75-250 students.
- Graduate physical organic chemistry: Chem 552.
- Freshmen seminar series: Chem 195.

TEACHING INNOVATION

- **Creator of Chem 357, Industrial Organic Chemistry.** This one-semester organic chemistry course replaced the typical two semester course chemical engineering majors. It teaches core organic chemistry principles of bonding, thermodynamics, reactive intermediates, and reaction mechanisms with an emphasis on industrial commodity chemistry processes. This is the first genuine industrial organic course offered to undergraduate students in the US.
- **Creator of Chem 195, Freshmen Seminar Series.** I created a course for freshmen chemistry majors. Chemistry 195 is designed to give freshmen an overview of all the divisions of traditional chemistry and their interface with biology, medicine, engineering, and other physical sciences. This class is a once a week seminar series. Speakers consist of either BYU professors, external industrial chemists, and professional speakers. This seminar series covers non-traditional employment, such as patent law and start-up companies.
- **Creator of Chem 397R, Mentored Service and Outreach.** This course is used to train BYU undergraduate students as Chem Camp counselors to teach children and youth science.

EXTERNAL SERVICE HIGHLIGHTS

- Guest editor for *Chemical Reviews* Volume 119, Issue 11 on “Computational Design of Catalysts from Molecules to Materials”. Authored editorial: <https://doi.org/10.1021/acs.chemrev.9b00296>.
- Cofounder of monthly Zoom conference computational chemistry conference (2020-present). Currently attended by >10 international research groups.
- Cofounder of annual “Utah Inorganometallic Conference” (2014-2019). Attended by BYU, UofU, and Utah State.

BYU AWARDS

- Karl G. Maeser Research and Creative Arts Award (2019)
- Richard Roskelly Teaching and Learning Fellowship (2017-2018)
- BYU Young Scholar Award (2015)
- BYU College of Physical and Mathematical Sciences Young Scholar Award (2014)

BYU COMMITTEES

Chair of undergraduate research awards	2012-2015
Chair of graduate recruiting	2015-2020

MENTORED POSTDOCS

Dr. Justin Kirkland (Jan. 2021-present)
Dr. Maliheh Tameh (Jan. 2021-present)
Dr. Shusen Chen (Aug. 2020-present)
Dr. Bo Yang (Oct. 2019-present)
Dr. Steven Maley (Jan. 2019-Nov. 2020)
Dr. Madhu Samolia (May 2019-Dec. 2019)
Dr. Jian Wang (Jan. 2015-Dec. 2015)
Dr. Deep Devarajan (Jan. 2014-Dec. 2015)
Dr. Alban Petit (Jan. 2013-July 2014)

MENTORED GRADUATE STUDENTS

Michael Davenport (June 2020-present)
Joshua Wheeler (June 2018-present)
Ryan Carlsen (May 2015-Aug. 2021)
James Coombs (Sept. 2018-Aug. 2021)

Dr. Doo-Hyun Kwon, Ph.D. (June 2014-June 2019) *Employed as computational chemist at GlaxoSmithKline.*

Dr. Clinton King, Ph.D. (Sept. 2014-Aug. 2019) *Employed as assistant professor at Utah Valley University.*

Jack Fuller, M.S. (June 2014-Aug. 2016) *Ph.D. student at UCLA.*

Dr. Samantha Gustafson, Ph.D. (Sept. 2011-Aug. 2016)

Jointly Advised Graduate Students:

Kyle Clark (June 2018-present) Jointly advising with Matthew Asplund and David Michaelis.

Dr. Ying Zhang, Ph.D. (Sept. 2013-July 2018) Jointly advised with Prof. Brian Woodfield. *Employed at Micron Inc.*

BYU PUBLICATION STATISTICS & HIGHLIGHTS

- h-index = 40; i10-index = 86 (Google Scholar for all publications on 11/08/2020)
- Total publications = 134
- BYU publications = 103
- Total senior author/corresponding author publications = 76
- *Science* publications = 3
- Publications with impact factor >8 = 35
- Publications with graduate students = 38
- Publications with undergraduate coauthors = 33

ISSUED PATENTS

4. Bischof, S. M.; Kilgore, U. J.; Sydora, O. L.; Ess, D. H.; Fuller, III, J. T.; Kwon, D.-H. “Fluorinated N₂-Phosphinyl Amidine Compounds, Chromium Salt Complexes, Catalyst Systems, and Their Use to Oligomerize Ethylene” (with Chevron Phillips Chem. Co. LP) US 10,493,442 B2. Issued 12/03/2019.

3. Bischof, S. M.; Kilgore, U. J.; Sydora, O. L.; Ess, D. H.; Fuller, III, J. T.; Kwon, D.-H. “Carbonyl-Ctaoning Perfluorohydrocarbyl-N²-Phosphinylamide Compounds, Chromium Salt Complexes and their use to Oligomerize Ethylene” (with Chevron Phillips Chem. Co. LP) US 10,294,171 B2. Issued 05/21/2019.

2. Bischof, S. M.; Kilgore, U. J.; Sydora, O. L.; Ess, D. H.; Fuller, III, J. T.; Kwon, D.-H. “Perfluorohydrocarbyl-N₂-Phosphinyl Amidine Compounds, Chromium Salt Complexes, Catalyst Systems, and Their Use to Oligomerize Ethylene” (with Chevron Phillips Chem. Co. LP) US 10,183,960 B1. Issued 01/22/2019.

1. Ess, D. H.; Falck, J. R. Jat, J. L. Kürti, L. “Direct Stereospecific Synthesis of Unprotected Aziridines from Olefins” US 9,988,349 B2. Issued 06/05/2018.

BYU PUBLICATIONS

(* = corresponding or co-corresponding author; ^Δ = undergraduate co-author from my lab)

141. Teynor, M. S.^Δ; Scott, W.^Δ; Ess, D. H.* “Catalysis with a Skip: Dynamically Coupled Addition, Proton Transfer, and Elimination during Au- and Pd-Catalyzed Diol Cyclizations” *ACS Catal.* **2021**, *11*, ASAP. <https://doi.org/10.1021/acscatal.1c02408>

140. Ence, C. C.; Martinez, E. E.; Himes, S. R.^Δ; Nazari, S. H.; Moreno, M. R.; Matu, M. F.; Larsen, S. G.; Gassaway, K. J.; Valdivia-Berroeta, G. A.; Smith, S. J.; Ess, D. H.*; Michaelis, D. J. “Experiment and

Theory of Bimetallic Pd-Catalyzed α -Arylation and Annulation for Naphthalene Synthesis” *ACS Catal.* **2021**, *11*, ASAP.

139. Davis, J. T.; Martinez, E. E.; Clark, K. J.; Kwon, D-H.; Talley, M. R.; Michaelis, D. J.; Ess, D. H.*; Asplund, M. C. “Time-Resolved Ultraviolet–Infrared Experiments Suggest Fe–Cu Dinuclear Arene Borylation Catalyst Can Be Photoactivated” *Organometallics* **2021**, *40*, 1859–1865.

<https://pubs.acs.org/doi/10.1021/acs.organomet.1c00136>

138. Yang, B.; Wheeler, J. I.; Sorensen, B.^Δ; Steagall, R.^Δ; Nielson, T.^Δ; Yao, J.; Mendez-Arroyo, J.; Ess, D. H.* “Computational Determination of Coordination Structure Impact on Adsorption and Acidity of Pristine and Sulfated MOF-808” *Mater. Adv.* **2021**, *2*, 4246–4254.

<https://pubs.rsc.org/en/content/articlehtml/2021/ma/d1ma00330e>

137. Yang, B.; Schouten, A.^Δ; Ess, D. H.* “Direct Dynamics Trajectories Reveal Nonstatistical Coordination Intermediates and Demonstrate that σ and π -Coordination Are Not Required for Rhenium(I)-Mediated Ethylene C–H Activation” *J. Am. Chem. Soc.* **2021**, 8367–8374.

<https://pubs.acs.org/doi/10.1021/jacs.1c01709>

136. Maley, S. M.; Melville, J.^Δ; Yu, S.^Δ; Teynor, M. S.^Δ; Carlsen, R.; Hargis, C.^Δ; Hamilton, R. S.^Δ; Grant, B. O.^Δ; Ess, D. H.* “Machine Learning Classification of Disrotatory IRC and Conrotatory Non-IRC Trajectory Motion for Cyclopropyl Radical Ring Opening” *Phys. Chem. Chem. Phys.* **2021**, *23*, 12309–12320.

<https://pubs.rsc.org/en/content/articlelanding/2021/cp/d1cp00612f#!divAbstract>

135. Carlsen, R.; Maley, S. M.; Ess, D. H.* “Timing and Structures of σ -Bond Metathesis C–H Activation Reactions from Quasiclassical Direct Dynamics Simulations” *Organometallics*, **2021**, *40*, 1454–1465.

<https://doi.org/10.1021/acs.organomet.1c00102>

134. McGuire, K. L.; Smit, P.; Ess, D. H.; Hill, J. T.; Harrison, R. G.; Busath, D. D. “Mechanism and Kinetics of Copper Complexes Binding to the Influenza A M2 S31N and S31N/G34E Channels” *Biophysical Journal* **2021**, *120*, 168–177.

<https://doi.org/10.1101/2020.08.24.265165>

133. Patel, D. I.; Shah, D.; Roychowdhury, T.; Wheeler, J. I. Ess, D. H.; Hilfiker, J. N.; Linford, M. R. “Diphenylsiloxane–Dimethylsiloxane Copolymer: Optical Function from 191 – 1688 nm (0.735 – 6.491 eV) by Spectroscopic Ellipsometry” *Surface Science Spectra* **2020**, *27*, 026001.

<https://doi.org/10.1116/6.0000249>.

132. Smith, J. A.; Schouten, A.^Δ; Wilde, J. H.; Westendorff, K. S.; Dickie, D. A.; Ess, D. H.*; Harmen, W. D. “Experiments and Direct Dynamics Simulations Reveal a Network of Reaction Pathways for Tungsten η^2 -Arene - Aryl Hydride Equilibria” *J. Am. Chem. Soc.* **2020**, *142*, 16437–16454.

<https://doi.org/10.1021/jacs.0c08032>

131. Major, G. H.; Chapman, S. C.; Chapman, J. T.; Wheeler, J. I.; Chatterjee, S.; Cushman, C. V.; Ess, D. H.; Linford, M. R. “Spectroscopic Ellipsometry of SU-8 Photoresist from 190 – 1680 nm (0.740 – 6.50 eV)” *Surface and Interface Analysis*, **2021**, *53*, 5–31.

<https://doi.org/10.1002/sia.6867>

130. Smith, J. D.; Durrant, G.; Ess, D. H.; Gelfand, B. S.; Piers, W. E. “H/D Exchange Under Mild Conditions in Arenes and Unactivated Alkanes with C₆D₆ and D₂O Using Rigid, Electron-rich Iridium PCP Pincer Complexes” *Chem. Sci.* **2020**, *11*, 10705–10717.

<https://doi.org/10.1039/D0SC02694H>

129. Maley, S. M.; Kwon, D-H.; Rollins, N.^Δ; Stanley, J. C.^Δ; Sydora, O. L.; Bischof, S. M.; Ess, D. H.* “Quantum-Mechanical Transition-State Model Combined with Machine Learning Provides Catalyst Design Features for Selective Cr Olefin Oligomerization” *Chem. Sci.* **2020**, 9665-9674. <https://doi.org/10.1039/D0SC03552A>
128. Kwon, D-H.; Maley, S. M.; Stanley, J. C.^Δ; Sydora, O. L.; Bischof, S. M.; Ess, D. H.* “Why Less Coordination Provides Higher Reactivity Chromium Phosphinoamidine Ethylene Trimerization Catalysts” *ACS Catal.* **2020**, *10*, 9674-9683. <https://pubs.acs.org/doi/10.1021/acscatal.0c02595>
127. Martinez, E. A.; Jensen, C. A.; Larson, A. J. S.; Kenney, K. C.; Clark, K. J.; Nazari, S. H.; Valdivia-Berroeta, G. A.; Smith, S. J.; Ess, D. H.; Michaelis, D. J. “Monosubstituted, Anionic Imidazolyl Ligands from N-H NHC precursors and Their Activity in Pd-Catalyzed Cross-Coupling Reactions” *Adv. Synth. Catal.* **2020**, *362*, 2876-2881. <https://doi.org/10.1002/adsc.202000483>
126. Rollins, N.^Δ; Pugh, S. L.^Δ; Maley, S. M.; Grant, B. O.^Δ; Hamilton, S. R.^Δ; Teynor, M. S.^Δ; Carlsen, R.; Jenkins, J. R.^Δ; Ess, D. H.* “Machine Learning Analysis of Direct Dynamics Trajectory Outcomes for Thermal Deazetization of 2,3-Diazabicyclo[2.2.1]hept-2-ene” *J. Phys. Chem. A* **2020**, *124*, 4813-4826. <https://doi.org/10.1021/acs.jpca.9b10410>
125. Wheeler, J.; Carlsen, R.; Ess, D. H.* Mechanistic Molecular Motion of Transition-Metal Mediated β-Hydrogen Transfer: Quasiclassical Trajectories Reveal Dynamically Ballistic, Dynamically Unrelaxed, Two Step, and Concerted Mechanisms” *Dalton Trans.* **2020**, *49*, 7747-7757. <https://doi.org/10.1039/D0DT01687J>
124. Gunsalus, N.; Koppaka, A.; Hashiguchi, B.; Konnick, M.; Park, S. H.; Ess, D. H.; Periana, R. “S_N2 and E2 Branching of Main-Group Metal Alkyl Intermediate in Alkane CH Oxidation: A Mechanistic Investigation using Isotopically Labelled Main-Group Metal Alkyls” Submitted. *Organometallics*, **2020**, *39*, 1907-1916. <https://doi.org/10.1021/acs.organomet.0c00120>
123. Avval, T. G.; Hodges, G. T.; Wheeler, J.; Ess, D. H.; Bahr, S.; Dietrich, P.; Meyer, M.; Thißen, A.; Linford, M. R. “Polyethylene terephthalate by near-ambient pressure XPS” *Surface Science Spectra*, **2020**, *27*, 014006. <https://doi.org/10.1116/1.5129466>
122. Teynor, M. S.^Δ; Carlsen, R.; Ess, D. H.* “Relationship Between Energy Landscape Shape and Dynamics Trajectory Outcomes for Methane C-H Activation by Cationic Cp*(PMe₃)Ir/Rh/Co(CH₃)” *Organometallics*, **2020**, *39*, 1393-1403. <https://doi.org/10.1021/acs.organomet.0c00108>
121. Macaulay, C. P.; Samolia, M.; Ferguson, M. J.; Sydora, O. L.; Ess, D. H.*; Stradiotto, M.; Turculet, L. “Synthetic Investigations of Low-Coordinate (N-Phosphino-amidinate) Nickel Chemistry: Agostic Alkyl Complexes and Benzene Insertion into Ni-H” *Dalton Trans.* **2020**, *49*, 4811-4816. <https://doi.org/10.1039/D0DT00527D>
120. Cheng, Q-Q.; Zhou, Z.; Jiang, H.; Siitonen, J. H.; Ess, D. H.; Zhang, X.; Kürti, L. “Organocatalytic nitrogen transfer to unactivated olefins via transient oxaziridines” *Nat. Cat.* **2020**, *3*, 386–392. <https://doi.org/10.1038/s41929-020-0430-4>
119. Johnson, B. I.; Avval, T. G.; Wheeler, J. J.; Anderson, H. C.; Diwan, A.; Stowers, K. J.; Ess, D. H.; Linford, M. R. “Semiempirical Peak Fitting Guided by Ab Initio Calculations of X-ray Photoelectron Spectroscopy Narrow Scans of Chemisorbed, Fluorinated Silanes” *Langmuir*, **2020**, *36*, 1878-1886. <https://doi.org/10.1021/acs.langmuir.9b03136>

118. King, C. R.; Holdaway, A.^Δ; Durrant, G.^Δ; Wheeler, J.; Suaava, L.; Konnick, M. M.; Periana, R. A.; Ess, D. H.* “Supermetal: SbF₅-Mediated Methane Oxidation Occurs by C-H Activation and Isobutane Oxidation Occurs by Hydride Transfer” *Dalton Trans.* **2019**, *48*, 17029-17036. <https://doi.org/10.1039/C9DT03564H>
117. Aoki, Y.; Bauer, M.; Braun, T.; Cadge, J. Davies, D.; Durand, D.; Eisenstein, O.; Ess, D.; Fairlamb, I.; Fey, N.; Gallarati, S.; George, M.; Greaves, M.; Halse, M.; Hamilton, A.; Harvey, J.; Haynes, A.; Hintermair, U.; Hulme, A.; Ishii, Y.; Jakoobi, M.; Jensen, V. R.; Kennepohl, P.; Kuwata, S.; Lei, A.; Lloyd-Jones, G.; Love, J.; Lovelock, K.; Lynam, J.; Macgregor, S.; Marder, T.; Meijer, E. J.; Morgan, P.; Morris, R.; Mwansa, J.; Nelson, D.; Odom, A.; Perutz, R.; Reiher, M.; Renny, J.; Roithová, J.; Schafer, L.; Schilter, D.; Scott, S.; Slattery, J.; Walton, J.; Wilden, J.; Wong, C.-Y.; Yaman, T. “Physical methods for mechanistic understanding: general discussion” *Faraday Discussions*, **2019**, *220*, 144-178. <https://doi.org/10.1039/C9FD90070E>
116. Bauer, M.; Cadge, J.; Davies, D.; Durand, D.; Eisenstein, O.; Ess, D.; Fey, N.; Gallarati, S.; George, M.; Hamilton, A.; Harvey, J.; Hintermair, U.; Hulme, A.; Ishii, Y.; Jensen, V. R.; Lloyd-Jones, G.; Love, J.; Lynam, J.; Macgregor, S.; Marder, T.; Meijer, E. J.; Morgan, P.; Morris, R.; Mwansa, J.; Odom, A.; Perutz, R.; Reiher, M.; Schafer, L.; Slattery, J.; Young, T. “Computational and theoretical approaches for mechanistic understanding: general discussion” *Faraday Discussions*, **2019**, *220*, 464-488. <https://doi.org/10.1039/C9FD90073J>
115. Jain, V.; Wheeler, J. J. Ess, D. H.; Noack, S.; Vacogne, C. D.; Schlaad, H.; Bahr, S.; Dietrich, P.; Meyer, M.; Thißen A.; Linfoord, M. R. “Poly(γ -benzyl L-glutamate), by near-ambient pressure XPS” *Surface Science Spectra* **2019**, *26*, 024010. <https://doi.org/10.1116/1.5109121>
114. Carlsen, R.; Jenkins, J. R.^Δ; Ess, D. H.* “Molecular Dynamics Analysis of the Cationic Cp*(PMe₃)Ir(CH₃) Methane C-H Activation Mechanism” *Faraday Discussions*, **2019**, *220*, 414-424. <https://doi.org/10.1039/C9FD00035F>
113. Ess, D. H.*; Gagliardi, L.; Hammes-Schiffer, S. “Introduction: Computational Design of Catalysts from Molecules to Materials” *Chem. Rev.* **2019**, *119*, 6507-6508. <https://doi.org/10.1021/acs.chemrev.9b00296>
112. Gunsalus, N. J.; Park, S. H.; Hashiguchi, B. G.; Koppaka, A.; Smith, S. J.; Ess, D. H.*; Periana, R. A. “Selective N Functionalization of Methane and Ethane to Aminated Derivatives by Main-Group-Directed C-H Activation” *Organometallics* **2019**, *38*, 2319-2322. <https://doi.org/10.1021/acs.organomet.9b00246>
111. Ahn, S.; Hong, M.; Sundararajan, M.; Ess, D. H.*; Baik, M-H. “Design and Optimization of Catalysts Based on Mechanistic Insights Derived from Quantum Chemical Reaction Modeling” *Chem. Rev.* **2019**, *119*, 6509-6560. <https://doi.org/10.1021/acs.chemrev.9b00073>
110. Kattamuri, P.; Bhakta, U.; Siriwongsup, S.; Kwon, D-H.; Alemany, L.; Yousufuddin, M.; Ess, D. H.; Kürti, L. “Synthesis of Structurally Diverse 3-, 4-, 5- and 6-Membered Heterocycles from Diisopropyl Iminomalonates and Soft C-Nucleophiles” *J. Org. Chem.* **2019**, *84*, 7066-7099. <https://doi.org/10.1021/acs.joc.9b00681>

109. Carlsen, R.; Jenkins, J. R.^Δ; Chuang, J.^Δ; Pugh, S. L.^Δ; Ess, D. H.* “Paddle Ball Dynamics During Rh-Methyl to Rh-Methane σ -Complex Reductive Elimination” *Organometallics* **2019**, *38*, 2280-2287. <https://doi.org/10.1021/acs.organomet.8b00936> Cover of Issue 10: <https://pubs.acs.org/toc/orgnd7/38/10>.
108. Cloutier, J-P.; Rechinat, L.; Canac, Y.; Ess, D. H.*; Zargarian, D. “C-O and C-N Functionalization of Cationic, NCN-Type Pincer Complexes of Trivalent Nickel: Mechanism, Selectivity, and Kinetic Isotope Effect” *Inorg. Chem.* **2019**, *58*, 3861-3874. <https://doi.org/10.1021/acs.inorgchem.8b03489>
107. Zhang, Y.; Karunananda, M.; Williams, W.^Δ; Clark, K.; Mankad, N.; Ess, D. H.* “Dynamically Bifurcating Hydride Transfer Mechanism and Origin of Inverse Kinetic Isotope Effect for Heterodinuclear AgRu-Catalyzed Alkyne Semi-Hydrogenation” *ACS Catal.* **2019**, *9*, 2657-2663. <https://doi.org/10.1021/acscatal.8b04130>
106. Koppaka, A.; Park, S. H.; Hashiguchi, B. G.; Gunsalus, N. J.; King, C. R.; Konnick, M. M.; Ess, D. H.*; Periana, R. A. “Selective C-H Functionalization of Methane and Ethane by a Molecular Sb(V) Complex” *Angew. Chem. Int. Ed.* **2019**, *58*, 2241-2245. <https://doi.org/10.1002/anie.201809159>
105. Kwon, D-H.; Small, B.; Sydroa, O. L.; Bischof, S. M.; Ess, D. H.* “The Challenge of Using Practical DFT to Model Fe Pendant Donor Diimine Catalyzed Ethylene Oligomerization” *J. Phys. Chem. B* **2019**, *123*, 3727-3739. <https://doi.org/10.1021/acs.jpcc.9b00129>
104. Ess, D. H.* “Rapid Enantioselective Catalyst Optimization” *Nature Catalysis* **2019**, *2*, 8-9. <https://doi.org/10.1038/s41929-018-0216-0>
103. Cardon, J. M.; Coombs, J. C.; Ess, D. H. Castle, S. L. “Insights into base-free OsO₄-catalyzed aminohydroxylations employing chiral ligands” *Tetrahedron* **2019**, *75*, 945-948. <https://doi.org/10.1016/j.tet.2019.01.018>
102. Behnke, N.; Kielawa, R.; Kwon, D-H.; Ess, D. H.; Kürti, L. “Direct Primary Amination of Alkylmetals with NH-Oxaziridine” *Org. Lett.* **2018**, *20*, 8064-8068. <https://doi.org/10.1021/acs.orglett.8b03734>
101. Coombs, J.^Δ; Perry, D.; Kwon, D-H.; Thomas, C. M.; Ess, D. H.* “Why Two Metals Are Better Than One for Cobalt Phosphinoamide Catalyzed Kumada Coupling” *Organometallics* **2018**, *37*, 4195-4203. <https://doi.org/10.1021/acs.organomet.8b00449>
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LIST OF MENTORED UNDERGRADUATE STUDENTS

❖ All students mentored >1 year

Brian Kirk (2010-2013)

Corey S. Ellis (2010-2012)

Preston Stewart (2010-2012)

Melinda Lambert (2010-2011)

Alex Miller (2011-2012)
Kevin Jenson (2011-2012)
Thomas Cook (2011-2013)
Pete J. Anderson (2011-2013)
Josh Flygare (2011-2013)
Gerrit Winkel (2011-2012)
Michael Devonas (2011-2014)
Austin Talbot (2011- 2015)
Krissie Bak (2011-2012)
Brendan Leach (2012-2013)
Benjamin Kay (2012-2015)
Scott Michaelis (2013-2014)
Sam Roberts (2013-2015)
Josh Reitz (2013-2014)
Austin Jacobs (2013-2014)
Ben Black (2014-2015)
Sergio Mendoza (2014-2016)
Steven Butler (2014-2016)
Matt Proctor (2014-2016)
Nathan Wohlgemuth (2014-2017)
Justin Snyder (2014-2016)
Steven Jones (2015-2016)
Chance Clinger (2015-2016)
Jimmy Coombs (2015-2017)
Kayla Bixler (2016-2017)
Lily Hamill (2016-2018)
Dalton Perry (2016-2018)
Wendy Williams (2016-2018)
Ashley Holdaway (2017-2019)
Wendy Juo-Chun (2017-2018)

Nick Rollins (2017-2019)
Johnathan Stanley (2017-2020)
Johnny Huang (2017-2020)
Anna Schouten (2018-2020)
Cam Jackson (2018-2019)
Samuel Pugh (2018-2020)
Jordan Jenkins (2018-2019)
Kavika Faleumu (2018-2019)
Ernest Puleasi (Summer REU 2018)
Alexander Gibson (2018-2019)
Robert Steagall (2019-)
Matthew Teynor (2019-)
Hector Torress (Summer REU 2019)
Lorna Suaava (Summer REU 2019)
Taylor Nielson (2019-)
Brett Sorensen (2019-)
Nathan Morgan (2019-)
Windsor Scott (2019-)
Ian Abrams (2019-)
Cal Hargis (2020-)
Benjamin Grant (2020-)
Reid Spencer Hamilton (2020-)
Jessie Melville (2020-)
Michal Gibson (2020-)
Elayna Zalit (2020-)
Spencer Yu (2020-)
Gabriel Reed (2020-)
James Monson (2020-)
Mason Brown (Summer Talmage 2020)
Billy Hirschi (2020-)