DANIEL H. ESS

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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 Comp. Inorganic	University of North Carolina at Chapel Hill (10/09-6/10) Advisors: Cynthia K. Schauer and Thomas J. Meyer
Postdoctoral Scholar Comp. & Experimental Catalysis	The Scripps Research Institute, Florida (10/07-10/09) Advisor: Roy A. Periana California Institute of Technology (10/07-10/09) Advisor: William A. Goddard, III

CURRENT FUNDED RESEARCH AREAS

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

CURRENT AWARDS (Total for all awards ~4,000,000)

- *National Science Foundation*, "Theory and Design of Dinuclear Catalytic Reactions" CHE-2153215 (PI, 2022-2025)
- *DOD: Army Research Laboratory*, "CLES-EM: Clean, Lean, and Efficient Synthesis of Energetic Materials" Rice-Army Cooperative Agreement (subcontract, 2021-2026)
- *National Science Foundation*, "Collaborative Research: Improving Student Learning in Organic Chemistry Using Chemical Reaction Simulations" DUE-2121023 (PI, 2021-2024)
- *National Institutes of Health, NIGMS*, "Nickel Catalyzed Electrochemical C-C Cross-Coupling Reactions" 1R15GM143721-01 (subcontract, 2021-2024)
- *National Science Foundation*, "Dynamical Organometallic Mechanisms" CHE-1952420 (PI, 2020-2023)
- *Chevron Phillips Chemical Co.*, "Design of Homogeneous Catalysts" (PI, 2014-2022)
- *Phillips 66*, "Computational Optimization of Acids" (PI, 2019-2022)

- *National Science Foundation*, "Chemistry and Biochemistry REU Site to Prepare Students for Graduate School and an Industrial Career" CHE-1757627 (PI, 2018-2021); 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 azirdinations and ring-opening transformations" 1R35GM136373-01 (subcontract, 2020-2025)

COMPLETED AWARDS

- *National Science Foundation*, "Theory and Design of Transition-Metal Heterodinuclear and Homodinuclear Catalytic Reactions" CHE-1764194 (PI, 2018-2021)
- *National Institutes of Health, NIGMS*, "Asymmetric N-H/N-alkyl olefin azirdinations 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 DEVEOPMENT

https://github.com/DanielEss-lab

- **Milo:** A quasiclassical direct dynamics program.
- **Mason and Taylor:** Automated construction and optimization of molecular transition-state structures.
- **MECPro:** Efficient program to locate minimum energy crossing points.

CHEMISTRY CAMPS

- Creator and co-director of BYU Chem Camp for children ages 9-12 (https://chemcamp.byu.edu/9-12) >400 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 (2020-2021). Currently attended by >10 international research groups.
- Cofounder of annual "Utah Inorganometallic Conference" (2014-2019). Attended by BYU, UofU, and Utah State.
- Reviewer of >300 journal articles. Example of journals are: *Science, Nature, Nature Chemistry, Nature Catalysis, Journal of the American Chemical Society, Chemical Science, ACS Catalysis, Inorganic Chemistry, Journal of Physical Chemistry, and Organometallics.*
- Panel and "mail-in" grant review. Examples include Department of Energy, National Science Foundation, and Petroleum Research Foundation.

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. Jyothish Joy (Jan. 2022-present)
Dr. Jugal Kumawat (Jan. 2022-present)
Dr. Justin Kirkland (Jan. 2021-present)
Dr. Shusen Chen (Aug. 2020-present)
Dr. Bo Yang (Oct. 2019-present)
Dr. Maliheh Tameh (Jan. 2021-Jan. 2022)
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)
Dr. Ryan Carlsen, Ph.D. (May 2015-Aug. 2021) *Employed as chemistry teacher at Logan High School*
James Coombs (Sept. 2018-Dec. 2020)
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:
Artem Marchenko (Jan. 2022-present) Jointly advising with David Michaelis
Kyle Clark (June 2018-Apr. 2020) 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 = 44; i10-index = 93 (Google Scholar for all publications on 01/19/2022)
- Total publications = 148
- BYU publications = 117

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 Perflurohydrocarbyl-N^2-Phosphinylamizde 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; $^{\Delta}$ = undergraduate co-author from my lab)

150. Kattamuri, P. V.; Siitonen, J. H.; Morgan, N.; Ess, D. H.* Kürti, L. Aza-Quasi-Favorskii: Construction of Highly Substituted Aziridines Through a Concerted Multi-bond Rearrangement Process. *J. Am. Chem. Soc. Accepted*.

149. Maley, S. M.; Lief, G. R.; Buck, R. M.; Sydora, O. L.; Yang, Q.; Bischof, S. M.; Ess, D. H.* DFT and CCSD(T) Evaluation of Ionization Potentials, Redox Potentials, and Bond Energies Related to Zirconocene Polymerization Catalysts. *J. Comput. Chem. Accepted*.

148. Maley, S. M.; Steagall, R.[Δ]; Lief, G. R.; Buck, R. M.; Yang, Q.; Sydora, O. L.; Bischof, S. M.; Ess, D. H.* Computational Evaluation and Design of Polyethylene Zirconocene Catalysts with Noncovalent Dispersion Interactions. *Organometallics*, **2022**, *41*, 581-593. https://pubs.acs.org/doi/full/10.1021/acs.organomet.1c00670

147. Clapson, M. L.; Kirkland, J. K.; Piers, W. E.; Ess, D. H.*; Gelfand, B.; Lin, J.-B. Carbene Character in a Series of Neutral $PC_{carbene}P$ Cobalt(I) Complexes: Radical Carbenes Versus Nucleophilic Carbenes *Organometallics*, **2022**, 41, 235-245. https://pubs.acs.org/doi/10.1021/acs.organomet.1c00585

146. Morgan, N.[Δ]; Maley, S. M.; Kwon, D-H.; Webster-Gardiner, M. S.; Small, B. L.; Sydora, O. L.; Bischof, S. M. Ess, D. H.* Computational Assessment and Understanding of C_6 Product Selectivity for Chromium Phosphinoamidine Catalyzed Ethylene Trimerization. *J. Organometallic Chem.* **2022**, *961*, 122251. https://www.sciencedirect.com/science/article/pii/S0022328X21005726

145. Chen, S.; Nielson, T.; Zalit, E.; Skjelstad, B. B.; Borough, B.; Hirschi, W. J.; Yu, S.; Balcells, D. Ess, D. H.* Automated Construction and Optimization Combined with Machine Learning to Generate Pt(II) Methane C–H Activation Transition States. *Topics in Catalysis* **2022**, 65, 312-324. https://doi.org/10.1007/s11244-021-01506-0

144. Ess, D. H.* Quasiclassical Direct Dynamics Trajectory Simulations of Organometallic Reactions. *Acc. Chem. Res.* **2021**, *54*, 4410-4422. https://doi.org/10.1021/acs.accounts.1c00575

143. Steiman, T. J.; Kalab, A. E.; Coombs, J. C.; Kirkland, J. K.; Torres, H.[Δ]; Ess, D. H.; Uyeda, C. Dinickel-Catalyzed Vinylidene–Alkene Cyclization Reactions. *ACS Catal.*, **2021**, *11*, 14408-14416. https://doi.org/10.1021/acscatal.1c03350

142. Chen, S-S.; Koppaka, Anjaneyulu, Periana, R. A.; Ess, D. H.* Theory and Experiment Demonstrate that Sb(V)-Promoted Methane C-H Activation and Functionalization Outcompetes Superacid Protonolysis in Sulfuric Acid. *J. Am. Chem. Soc.* **2021**, *143*, 18242-18250. https://doi.org/10.1021/jacs.1c08170

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*, 10179-10189. 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*, 10394-10404. https://pubs.acs.org/doi/full/10.1021/acscatal.1c02731

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 C_6D_6 and D_2O 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.$^{\Delta}$; Pugh, S. L.$^{\Delta}$; Maley, S. M.; Grant, B. O.$^{\Delta}$; Hamilton, S. R.$^{\Delta}$; Teynor, M. S.$^{\Delta}$; Carlsen, R.; Jenkins, J. R.$^{\Delta}$, 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. *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.; Thiβen, 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.$^{\Delta}$; Carlsen, R.; Ess, D. H.* Relationship Between Energy Landscape Shape and Dynamics Trajectory Outcomes for Methane C-H Activation by Cationic Cp*(PMe_3)Ir/Rh/Co(CH_3). *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.$^{\Delta}$; Durrant, G.$^{\Delta}$; Wheeler, J.; Suaava, L.; Konnick, M. M.; Periana, R. A.; Ess, D. H.* Supermetal: SbF_5-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.; Linford, 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*(PMe_3)Ir(CH_3) 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

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LIST OF MENTORED UNDERGRADUATE STUDENTS

- All students mentored >1 year

Brian Kirk (2010-2013)
Preston Stewart (2010-2012)
Corey S. Ellis (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 Puletasi (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 (2019-2021)
Brett Sorensen (2019-2020)
Nathan Morgan (2019-2022)
Windsor Scott (2019-2020)
Ian Abrams (2019)
Cal Hargis (2020-)
Benjamin Grant (2020-2021)
Reid Spencer Hamilton (2020-2022)
Jessie Melville (2020-)
Elayna Zalit (2020-)
Spencer Yu (2020-2021)
Gabriel Reed (2020)
James Monson (2020)
Mason Brown (Summer Talmage 2020)
Billy Hirschi (2020-)
Jeremiah Brown (2021-)
Braden Borough (2021-2022)
Zack Meyer (2021-)
David Hawley (2021-2022)
Jared Rossberg (2021-)
Brendan Jensen (2022-)
Drew Hartsfield (2022-)
Nathan Todd (2022-)
Ishmael Taleo (2022-)
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Aidan Goble (2022-)
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