DANIEL H. ESS

Professor
Department of Chemistry and Biochemistry
Brigham Young University
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EDUCATION

Ph.D. 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) Advisors: Cynthia K. Schauer and Thomas J. Meyer
Postdoctoral Scholar	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

RESEARCH AREAS

- Organometallic reaction dynamics simulations
- Computational catalyst design
- Computational and experimental hydrocarbon C-H functionalization reactions
- Computational studies of multinuclear transition-metal catalysis

CURRENT AWARDS (Total for all awards = $7,455,968)

- *National Science Foundation*, "Dynamic Effects Controlling Mechanisms and Selectivity in Transition Metal-Oxo Reactions" CHE-2555134 (PI, 2026-2029)
- *National Institutes of Health, NIGMS*, "Modeling Multimetallic Transition Metal Catalysts to Enhance Organic Synthesis" 1R15GM163265-01 (PI, 2026-2029)
- *U.S. Department of Energy, Office of Basic Energy Sciences, Catalysis Sciences*, "Theory of Main-Group, p-Block Hydrocarbon Functionalization Reactions" DE-SC0018329 (PI, 2017-2020) and renewals "Modeling and Design of Main-Group Metal Catalyzed Alkane C-H Functionalization Reactions" (PI, 2020-2029)
- *National Science Foundation*, "GOALI: Computational, Data Science, and Synthetic Approach to the Design of Retro-Hydroformylation Catalysts" CHE-2452595 (PI, 2025-2028)
- *Chevron Phillips Chemical Co.*, "Design of Homogeneous Alpha Olefin Catalysts" (PI, 2014-2026)
- *American Chemical Society Petroleum Research Foundation*, "Design, Synthesis, and Testing of Molecular Catalysts for Direct and Selective Alkane Dehydrogenation" PRF #70613-ND3 (PI, 2026-2028)

- *Rice University/National Institutes of Health, NIGMS*, "New Frontiers in the Streamlined Synthesis of N-Unprotected Chiral Heterocycles and Amines via Organo- and Transition Metal Catalysis" 1R35GM161793-01 (subcontract, 2026-2027)

COMPLETED AWARDS

- *National Science Foundation*, "Dynamics of Organometallic Reaction Mechanisms" CHE-2244799 (PI, 2023-2026)
- *National Science Foundation*, "Theory and Design of Dinuclear Catalytic Reactions" CHE-2153215 (PI, 2022-2026)
- *Rice University/National Institutes of Health, NIGMS*, "Asymmetric N-H/N-alkyl olefin azirdinations and ring-opening transformations" 1R35GM136373-01 (subcontract, 2020-2025)
- *National Science Foundation*, "Collaborative Research: Improving Student Learning in Organic Chemistry Using Chemical Reaction Simulations" DUE-2121023 (PI, 2021-2024)
- *Utah State University/National Institutes of Health, NIGMS*, "Nickel Catalyzed Electrochemical C-C Cross-Coupling Reactions" 1R15GM143721-01 (subcontract, 2021-2024)
- *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
- *National Science Foundation*, "Dynamical Organometallic Mechanisms" CHE-1952420 (PI, 2020-2023)
- *Phillips 66*, "Computational Optimization of Solid Acid Metal-Organic Frameworks" (PI, 2019-2022)
- *Rice University/DOD: Army Research Laboratory*, "CLES-EM: Clean, Lean, and Efficient Synthesis of Energetic Materials" Rice-Army Cooperative Agreement (subcontract, 2021-2026)
- *National Science Foundation*, "Theory and Design of Transition-Metal Heterodinuclear and Homodinuclear Catalytic Reactions" CHE-1764194 (PI, 2018-2021)
- *UT Southwestern/Rice University/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 molecular dynamics program.
- **ReaLigands:** A library of experimental ligands for computational catalyst design.
- **Mason:** Automated construction and optimization of molecular transition-state structures.
- **MECPro:** Efficient program to locate minimum energy crossing points.
- **MOFseek:** Software that analyzes metal-organic framework structures.
- **iORA:** iPhone application that animates organic reaction direct dynamics simulations. Type "iORA" into the Apple App Store.
- **webORA:** http://webora.chem.byu.edu/

CHEMISTRY CAMPS

- >1,000 children/youth participants since 2016.

- Creator and co-director of BYU Chem & BioChem Camps for children ages 9-14 (https://chemcamp.byu.edu/).

SUMMER VISITING UNDERGRADUATE RESEARCH PROGRAM

- 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*". 2018-2024. This program hosted 10 visiting undergraduate students and two high school teachers to conduct summer research.

COURSES TAUGHT

- Organic chemistry 1 and 2: Chem 351, 351M, 352, 352M, and 357 (industrial organic). These are large section classes ranging from 75-250 students.
- Graduate physical organic chemistry: Chem 552.
- Graduate computational chemistry: Chem 596R.
- Mentored service and outreach: Chem 397R.
- Freshman 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.
- **Creator of Chem 397R**, Mentored Service and Outreach. This course is used to train BYU undergraduate students as Chem Camp counselors.

EXTERNAL SERVICE HIGHLIGHTS

- Guest editor for *J. Chem. Phys.* 2022, Volume 157, on "Chemical Design by Artificial Intelligence". Authored editorial: https://aip.scitation.org/doi/10.1063/5.0123281
- 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 "Utah Inorganometallic Conference" (2014-2019).

BYU AWARDS

- Roland K. Robins Department Graduate Teaching and Mentoring Award (2024)
- 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)

MENTORED POSTDOCS

Dr. Wang-Yeuk (Kevin) Kong (Sept. 2025-present)
Dr. Anjaneyulu Koppaka (Aug. 2024-present)
Dr. Kevin Quirion (July 2024-present)
Dr. Anthony Schaefer (July 2022-present)
Dr. Jyothish Joy (Jan. 2022-present)
Dr. Jugal Kumawat (Jan. 2022-Dec. 2024)
Dr. Olajumoke Dunsin (Jan. 2023-Dec. 2023)
Dr. Justin Kirkland (Jan. 2021-July 2023) Data Scientist
Dr. Shusen Chen (Aug. 2020-Aug. 2023) Assistant Professor, Chingqong University (China)

Dr. Bo Yang (Oct. 2019-Sept. 2022) Comp. Chemist, Eastman Chemical
Dr. Maliheh Tameh (Jan. 2021-Jan. 2022)
Dr. Steven Maley (Jan. 2019-Nov. 2020) Assistant Professor, Wilfrid Laurier University (Canada)
Dr. Madhu Samolia (May 2019-Dec. 2019) Assistant Professor, Chandigarh University, Mohali (India)
Dr. Jian Wang (Jan. 2015-Dec. 2015)
Dr. Deep Devarajan (Jan. 2014-Dec. 2015)
Dr. Alban Petit (Jan. 2013-July 2014)

MENTORED GRADUATE STUDENTS

Committee Chair:

Dillon Park (Sept. 2024-present)
Krishna Adhaduk (Sept. 2024-present)
Dongdong (Marcus) Yang (Nov. 2023-present)
Michael Davenport (June 2020-June 2025) *Computational chemist at AutoLiv*
Dr. Joshua Wheeler, Ph.D. (June 2018-July 2023) *Instructor Costal Carolina University*
Dr. Ryan Carlsen, Ph.D. (May 2015-Aug. 2021) *Postdoc at University of Utah*
James Coombs, (Sept. 2018-Dec. 2020) *High school teacher, Rifle Colorado*
Dr. Doo-Hyun Kwon, Ph.D. (June 2014-June 2019) *Computational chemist at Recursion Pharmaceuticals (previously at GlaxoSmithKline)*
Dr. Clinton King, Ph.D. (Sept. 2014-Aug. 2019) *Teaching Lab Manager (Organic) at Utah Valley University.*
Jack Fuller, M.S. (June 2014-Aug. 2016) *Ph.D. at UCLA; Postdoc at PNNL*
Dr. Samantha Gustafson, Ph.D. (Sept. 2011-Aug. 2016)

Jointly Advised Graduate Students:

Kyle Clark (June 2018-Apr. 2020) Jointly advised 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.*

MENTORED UNDERGRADUATE STUDENTS

Brian Kirk (2010-2013); Preston Stewart (2010-2012); Corey Ellis (2010-2012); Melinda Lambert (2010-2011); Alex Miller (2011-2012); Kevin Jenson (2011-2012); Thomas Cook (2011-2013); Pete 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 (2019-2021); Matthew Teynor (2019-2022); 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 (2020-2022); Benjamin Grant (2020-2021); Reid Spencer Hamilton (2020-2022); Jessie Melville (2020-2022); Elayna Zalit (2020-2023); Spencer Yu (2020-2021); Gabriel Reed (2020); James Monson (2020); Mason Brown (Summer 2020); Billy Hirschi (2020-2025); Jeremiah Brown (2021-2024); Braden Borough (2021-2022); Zack Meyer (2021-2023); David Hawley (2021-2022); Jared Rossberg (2021-2023); Brendan Jensen (2022-2023); Drew Hartsfield (2022-); Nathan Todd (2022-2023); Ishmael Taleo (2022); Allison Lambert (2022-2025); Ariana Carter (Summer REU 2022); Aidan

Goble (2022-2023); Alex Kraus (2022-2025); Trevor Mallavia (2022-2025); Iran Daniela Macias (2022-2023); Ty Showalter (2023); Tyson Tolman (2023-2024); Harlan Stevens (2023-2024); Eve Davis (2023-2024); Amber Abbott (2023); Josh Hansen (2023-2026); Spencer Ricks (2023-); Britton Stanley (2023-2025); Danny Manning (2023-); Caz Cullimore (2023-2024); Tyson Peterson (2023-2024); Julia Steed (2024); Lillian Woolston (2024-); Jonah Clark (2024-2026); Lydia Schouten (2024-); Isaac Smith (2024-2026); Conner Simmons (2024-2025); Henry Andrus (2024-2025); Alex Curtis (2025); Dallin Dunn (2025-); Nina Fullmer (2026-); Rebekah Windham (2026-); Mason Jones (2026-); Max David (2026-); Lincoln Frandsen (2026-); Barnabas Torok (2026-); Eli Atkinson (2027-)

BYU PUBLICATION STATISTICS & HIGHLIGHTS

- h-index = 53; i10-index = 152 (Google Scholar for all publications on 10/26/2026)

ISSUED PATENTS

11. Bischof, S. M.; Kilgore, U. J.; Sydora, O. L.; Ess, D. H. Kwon, D-H.; Rollins, N. K. Machine Learning and Statistical Analysis for Catalyst Structure Prediction and Design. (with Chevron Phillips Chem. Co. LP). US 12,102,992 B2. Issued 10/01/2024.

10. Bischof, S. M.; Sydora, O. L.; Ess, D. H. Modulating Co-Monomer Selectivity Using Non-Covalent Dispersion Interactions in Group 4 Olefin Polymerization Catalysts. (with Chevron Phillips Chem. Co. LP). US 11,859,041 B2. Issued 01/02/2024.

9. Bischof, S. M.; Sydora, O. L.; Ess, D. H.; Kilgore, U. J.; Kwon, D-H. Chromium Phosphinyl Hydroisoindole Amidine Complexes for Tetramerization of Ethylene. (with Chevron Phillips Chem. Co. LP). US 11,691,931 B2. Issued 07/4/2023.

8. Bischof, S. M.; Sydora, O. L.; Kilgore, U. J.; Ess, D. H.; Kwon, D-H. Chromium Bicyclic Phosphinyl Amidine Complexes for Tetramerization of Ethylene. (with Chevron Phillips Chem. Co. LP). US 11,685,701 B2. Issued 06/27/2023. (Continuation of US 11,505,513 Bl).

7. Bischof, S. M.; Sydora, O. L.; Kilgore, U. J.; Ess, D. H.; Kwon, D-H. Chromium Phosphinyl Isoindole Amidine Complexes for Tetramerization of Ethylene. (with Chevron Phillips Chem. Co. LP). US 11,583,843 Bl. Issued 02/21/2023.

6. Bischof, S. M.; Sydora, O. L.; Kilgore, U. J.; Ess, D. H.; Kwon, D-H. Chromium Bicyclic Phosphinyl Amidine Complexes for Tetramerization of Ethylene. (with Chevron Phillips Chem. Co. LP). US 11,505,513 Bl. Issued 11/22/2022.

5. Bischof, S. M.; Sydora, O. L.; Kilgore, U. J.; Ess, D. H.; Kwon, D-H. Chromium Phosphinyl Hydroisoindole Amidine Complexes for Tetramerization of Ethylene. (with Chevron Phillips Chem. Co. LP). US 11,492,305 Bl. Issued 11/08/2022.

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-Containing 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.

DISSERTATION

Ess, D. H. Quantum Mechanical Theory of Reactivity and Selectivity in Organic and Organometallic Reactions 2007, University of California, Los Angeles

BYU PUBLICATIONS

(* = corresponding or co-corresponding author; $^{\Delta}$ = undergraduate co-author from my lab)

213. Davenport, M. T.; Park, D. R.; Schaefer, A. J.; Shenvi, R.; Ess, D. H.* Role of Dynamics and Spin State Crossover in Metal-Hydride Hydrogen Atom Transfer (MHAT) and Electron Transfer in Transmetalation during Co-Ni Multimetallic Catalyzed Alkene Hydroarylation. *J. Am. Chem. Soc.* **2026**, *Accepted and in press*.

212. Hoque, M. A.; Gehman, Z. M.; Bastani, F.; Clark, J. G.; Quirion, K. P.; Jain, A.; Dickie, D. A.; Venkatesh, A.; Reinke, P.; Ess, D. H.*; Gunnoe, T. B. Ag(I) Induced C–C Reductive Elimination from Pt(II): Role of Ag(I) and Counteranion. *Organometallics*, **2026**, *45*, 2533-2545. https://doi.org/10.1021/acs.organomet.6c00318

211. Georg, M.; Kwon, Y-D.; Boeckle, M.; Yang, D.; Ess, D. H.; Kürti, L. Complex Fragment Coupling via O-Mesyl Hydroxylamines: Direct Conversion of Primary Amines to Electrophilic Aminating Agents. *J. Am. Chem. Soc.* **2026**, *148*, 43691-43700. https://doi.org/10.1021/jacs.6c14811

210. Koppaka, A.; Cullimore, C.$^{\Delta}$; Joy, J.; Kraus, A.$^{\Delta}$; Periana, R. A.; Ess, D. H.* Non-Radical Pathways Control Methane Sulfonation versus Oxygenation C-H Functionalization Selectivity with Hg(II) and Au(III) Catalysis. *Chem. Sci.* **2026**, *17*, 10762-10771. DOI: 10.1039/D6SC01628F

209. Miura-Akagi, P. M.; Ah-Tye, Y. J. H.; Clark, J. G.; Quirion, K. P.; Kong, W-Y.; Howard, M. P.; Balkwill, L. G.; Yoshida, W. Y.; Yap, G. P. A.; Rheingold, A. L.; Ess, D. H.*; Hughes, R. P.; Cain, M. F. Hydrodefluorination of a Fluorobenzene Equivalent by Harnessing a P(III)/Pd(II)–P(V)/Pd(0) Redox Couple Using a P–CF_3-Functionalized Benzazaphosphole. *Inorg. Chem.* **2026**, *65*, 10655-10671. https://pubs.acs.org/doi/10.1021/acs.inorgchem.6c00734

208. Joy, J.; Odogwu, D. A.; Atkins, I.; Goldscheitter, J. A.; Villarreal-Quiroga, G. H.; Koppaka, A.; Smith, S. J.; Small, B. L.; Leseberg, J. A.; Bischof, S. M.; Webster-Gardiner, M. S.; Michaelis, D. J.; Ess, D. H.* Computational, Data Science, and Experimental Evaluation and Design of Molecular Transfer Hydroformylation Catalysts. *Organometallics*, **2026**, *45,* 1022-1032. https://pubs.acs.org/doi/10.1021/acs.organomet.5c00504 *Journal Cover: https://pubs.acs.org/toc/orgnd7/45/9*

207. Quirion, K. P.; Kong, W-Y.; Stanley, B.$^{\Delta}$; Joy, J. Ess, D. H.* Density Functional Theory Surrogate Enables Fast and Broad Computational Evaluation of Homogeneous Transition Metal Catalytic Energy Landscapes. *ACS Catal.* **2026**, *16*, 8053-8066. https://pubs.acs.org/doi/full/10.1021/acscatal.5c09093 *ChemRxiv*, **2025**. https://doi.org/10.26434/chemrxiv-2025-z1s3s

206. Taylor, N. A.; Evenson, J. N.; Gassaway, N. J.; Richardson, E. L.; Joy, J.; Odogwu, D. A.; Chartrand, C. C.; Cole, R. J.; Larson, A. J. S.; Southern, A.; Villarreal-Quiroga, G. H.; Smith, S. J.; Ess, D. H.; Webster-Gardiner, M. S.; Leseberg, J. A.; Small, B. L.; Michaelis, D. J. Synthesis of Phosphino-iminoquinoline-Type Tridentate Ligands with a Tetrahydroacridine Core for Iron-Catalyzed Hydrosilylation. *Organometallics*, **2026**, *45*, 619-623. https://pubs.acs.org/doi/full/10.1021/acs.organomet.5c00501

205. Webber, C. K.; Alférez, M. G.; Bastani, F.; Kumawat, J.; Kong, F.; Gehman, Z. M.; Ou, X.; Dickie, D. A.; Ess, D. H.*; Reinke, P.; Gunnoe, T. B. Synthesis and Characterization of a Copper Complex Supported by a Z-type Sb^{V} Ligand: XPS and DFT Study of Electronic Structure. *Organometallics*, **2026**, *45*, 438-448. https://doi.org/10.1021/acs.organomet.5c00420

204. Noble, Kirt; Lam, T. L. Angus; Hansen, Joshua; Corey, James; Kelly, Tyler; Smith, Stacey; Ess, Daniel; Michaelis, David Synthesis, Structure, Bonding, and Ligand Exchange of a Bimetallic Rhodium(II,II) Dimetallocyclobutane Complex. *Organometallics*, **2026**, *45*, 236-240. https://doi.org/10.1021/acs.organomet.5c00417

203. Kraus, A.$^{\Delta}$; Koppaka, A.; Periana, R. A.; Ess, D. H.* Reactivity, Selectivity, and Mechanism of Bi(V) Promoted Methane C-H Functionalization in Concentrated Sulfuric Acid. *J. Organomet. Chem.* **2026**, *1050*, 124047. https://doi.org/10.1016/j.jorganchem.2026.124047

202. Kwon, Y-D.; Joaquin, D.; Davenport, M. T.; Olsen, J.$^{\Delta}$; Carpio, M.; Yousufuddin, M.; Ess, D. H.; Kürti, L. Polar-to-Radical Crossover in Catalyst-Free Olefin Halo-Hydroxylamination: A Direct Route to Multifunctional Electrophilic Hydroxylamines. *JACS Au*, **2026**, *6*, 521-533. https://doi.org/10.1021/jacsau.5c01471

201. Joy, J.; Ess, D. H.* Radical Clock Substrates Measure Nonstatistical Dynamical Effects in Cytochrome P450 Mediated C-H Functionalization Reactions. *J. Am. Chem. Soc.* **2026**, *148*, 1858-1871. https://doi.org/10.1021/jacs.5c19469

200. Quirion, K. P.; Ess, D. H.* Mechanism, Selectivity, and What Prevents Closure of the Catalytic Cycle for H_2 Reduction of CO_2 Promoted by a Heterodinuclear Zirconium-Iridium Complex. *Phys. Chem. Chem. Phys.* **2026**, *28*, 1549-1555. https://doi.org/10.1039/D5CP03791C

199. Schaefer, A. J.; Mallavia, T.$^{\Delta}$; Ess, D. H.* Dynamics-Based Transition States Reveal Solvent Cage Effect and S_N2 Transition State Motion in Lewis Acid Catalyzed Stereoselective Tertiary Alcohol Nucleophilic Substitution Reactions. *Chem. Sci.* **2025**, *16*, 21554-21561. https://doi.org/10.1039/D5SC05616K

198. Gardiner, S.; Dollinger, P.; Kovacic, F.; Pietruszka, J.; Ess, D. H.; Jaeger, K-E.; Schröder, G. F.; Della Corte, D. Resolution of physics and deep learning-based protein engineering filters: A case study with a lipase for industrial substrate hydrolysis. PLoS One 20(9): e0332409. https://doi.org/10.1371/journal.pone.0332409

197. Yang, D.; Davenport, M. T.; Joy, J.; Schaefer, A. J.; Ess, D. H.* Computational Evaluation of the σ-Complex Lifetime and Origin of the Inverse Kinetic Isotope Effect for Methane Reductive Elimination from Cationic $Cp_2Re(H)(CH_3)$ *Organometallics* **2025**, *44*, 2309-2318. https://pubs.acs.org/doi/10.1021/acs.organomet.5c00298

196. Joy, J.; Kraus, A.[Δ]; Ricks, S.[Δ]; Ess, D. H.* Pd–Methyl Bond Energy─Property Correlations, Noncorrelations, Machine Learning Models, and Application to Polymerization Catalysis. *Organometallics* **2025**, *44*, 1566-1575. https://doi.org/10.1021/acs.organomet.5c00135

195. Quirion, K. P.; Singh, R. P.; Mankad, N. P.; Ess, D. H.* $CpFe(CO)_2$ Radical Generated from Dinuclear $[CpFe(CO)_2]_2$ and Mononuclear $(Cp)(CO)_2Fe(H)$: Density Functional Theory Is Accurate for One, But Not Both. *J. Phys. Chem. A* **2025**, *129*, 8093-8100. https://pubs.acs.org/doi/full/10.1021/acs.jpca.5c03507

194. Kong, F.; Webber, C. K.; Kumawat, J.; Quirion, K. P.; Ou, X.; Dickie, D. A.; Ess, D. H.; Gunnoe, T. B. Covalent Bonding Between Ir and High-Oxidation State Sb Constrained by Quinoline Scaffolds. *Inorg. Chem.* **2025**, *64*, 16721-16727. https://pubs.acs.org/doi/10.1021/acs.inorgchem.5c02934

193. Ou, X.; Kong, F.; Quirion, K. P.; Webber, C. K.; Dickie, D. A.; Ess, D. H.; Gunnoe, T. B. Synthesis of Quinoline-Based Rh–Sb Complexes: Inhibition of Halide Transfer to Access a Rh→Sb Z-Type Interaction. *Organometallics* **2025**, *44*, 1639-1643. https://pubs.acs.org/doi/full/10.1021/acs.organomet.5c00187

192. Schaefer, A. J.; Joy, J.; Davenport, M. T.; Ess, D. H.* Dynamic Effects Influincing Mechanisms and Selectivity in Metal-Mediated Organometallic Reactions. *Organometallics* **2025**, *44*, 1603-1619. https://pubs.acs.org/doi/full/10.1021/acs.organomet.5c00162

191. Gee, J. C.; Fulbright, K. W.; Ess, D. H.; Joy, J. Kinetics of Double-Bond Isomerizations Among 1-Octene and *cis* and *trans* Linear Internal Octenes on Dry Amberlyst15 Catalyst: Adsorbed Alcohol Becomes an Active Site. *J. Phys. Org. Chem.* **2025**, *38*, e70026. https://doi.org/10.1002/poc.70026

190. Koppaka, A.; Chen, S-S.; Yang, D.; Marchenko, A.; Koumleh, S. M.; Michaelis, D. J.; Periana, R. A.; Ess, D. H.* Computational and experimental evidence for Sb(V) metal mediated C–H activation and oxidative functionalization of arenes. *Chem. Sci.* **2025**, *16*, 11058-11066. https://doi.org/10.1039/D5SC02048D

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