DANIEL H. ESS

Professor
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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 > $5M)

- *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 renewals "Modeling and Design of Main-Group Metal Catalyzed Alkane C-H Functionalization Reactions" (PI, 2020-2026) DE-SC0018329
- *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, 2022-2025)
- *Chevron Phillips Chemical Co.*, "Design of Homogeneous Alpha Olefin Catalysts" (PI, 2014-2024)
- *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*, "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*, "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)
- *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)
- *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.
- **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

- >800 children/youth participants since 2016.
- Creator and co-director of BYU Chem Camp for children ages 9-12 (https://chemcamp.byu.edu/9-12) >500 children from 2016-present.
- Creator and co-director of BYU BioChem Camp for youth ages 13-14. (https://chemcamp.byu.edu/13-14) >200 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". 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

- 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. Kevin Quirion (July 2024- present)
Dr. Anthony Schaefer (July 2022-present)
Dr. Jyothish Joy (Jan. 2022-present)
Dr. Jugal Kumawat (Jan. 2022-present)
Dr. Olajumoke Dunsin (Jan. 2023-Dec. 2023)
Dr. Justin Kirkland (Jan. 2021-July 2023) Data Scientist, Xantol
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)
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:

Dongdong (Marcus) Yang (Nov. 2023-present)
Michael Davenport (June 2020-present)
Dr. Joshua Wheeler, Ph.D. (June 2018-July 2023) *Instructor BYU-Idaho*
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) *Assistant professor 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.*

BYU PUBLICATION STATISTICS & HIGHLIGHTS

- h-index = 48; i10-index = 123 (Google Scholar for all publications on 06/29/2024)

ISSUED PATENTS

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. 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. 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. 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)

178. Rodriguez Treviño, A. M.; Pandiri, S.; Loch-Temzelides, P.; Pandiri, S.; Kirkland, J. K.; Davenport, M. T.; Aguinaga, U.; Yousufuddin, M.; Ess, D. H.; Kürti, L. Forging Structural Complexity: Diastereoselective Synthesis of Densely Substituted β-Lactams with Dual Functional Handles for Enhanced Core Modifications. *Chem. Sci. Advance Article*. https://chemrxiv.org/engage/chemrxiv/article-details/657b6a4d66c138172930a4b5; https://doi.org/10.1039/D4SC01513D

178. Webber, C. K.; Kong, F.; Kumawat, J.; Joy, J.; Richardson, E. K.; Siano, P.; Dickie, D. A.; Ess, D. H.*; Gunnoe, T. B. Synthesis of Quinoline-Based Pt−Sb Complexes with L- or Z-Type 2 Interaction: Ligand-Controlled Redox via Anion Transfer. *Organometallics*, **2024**, *XX*, ASAP. https://doi.org/10.1021/acs.organomet.4c00221

177. Luo, J.; Davenport, M. T.; Ess, D. H.*; Liu, T. L. Nickel-Catalyzed Electrochemical Cross-Electrophile $C(sp^2)$-$C(sp^3)$ Coupling via a Ni^{II} Aryl Amido Intermediate. *Angew. Chem. Int. Ed.* **2024**, *63*, e202407118. https://doi.org/10.1002/anie.202407118; 10.26434/chemrxiv-2023-pdw1d

176. Luo, J.; Davenport, M. T.; Ess, D. H.*; Liu, T. L. Electro/Ni Dual-Catalyzed Decarboxylative $C(sp^3)$−$C(sp^2)$ Cross-Coupling Reactions of Carboxylates and Aryl Bromide. *Angew. Chem. Int. Ed.* **2024**, *63*, e202403844. https://doi.org/10.1002/anie.202403844; 10.26434/chemrxiv-2023-8cm07

175. Wheeler, J. I.; Schaefer, A. J.; Ess, D. H.* Trajectory Based Time-Resolved Mechanism for Benzene Reductive Elimination from Cyclopentadienyl Mo/W Phenyl Hydride Complexes. *J. Phys. Chem. A.* **2024**, *128*, 4775-4786. https://doi.org/10.1021/acs.jpca.4c01788

174. Schaefer, A. J.; Ess, D. H.* Vibrational synchronization and its reaction pathway influence from an entropic intermediate in a dirhodium catalyzed allylic C–H activation/Cope rearrangement reaction. *Phys. Chem. Chem. Phys.* **2024**, *26*, 11386-11394. https://doi.org/10.1039/D4CP00657G

173. Mpaata, P.; Miller, C. R.; Bonsrah, D. K.; Camp, A. B.; Ballard, K. M.; Angelie, L.; Kirkland, J.; Joy, J.; Hirschi, W. J.$^{\Delta}$; Smith, S. J.; Ess, D. H.; Andrus, M. B. Intramolecular Heteroatom and Styryl Diels–Alder Reactions, Asymmetric Cycloadditions of Chiral 3-Phenylallyl Maleic Esters. *J. Org. Chem.* **2024**, *89*, 3883-3893. https://pubs.acs.org/doi/abs/10.1021/acs.joc.3c02725

172. Sinhababu, S.; Singh, R. P.; Radzhabov, M. R.; Kumawat, J.; Ess, D. H.; Mankad, N. P. Coordination-induced O-H/N-H bond weakening by a redox non-innocent, aluminum containing radical. *Nature Communications* **2024**, *15*, 1315. https://www.nature.com/articles/s41467-024-45721-1

171. Kirkland, J. K.; Kumawat, J.; Tameh, M. S.; Tolman, T.; Lambert, A. C.; Lief, G. R.; Yang, Q.; Ess, D. H.* Machine Learning Models for Predicting Zirconocene Properties and Barriers. *J. Chem. Inf. Model.* **2024**, *64*, 775-784. https://pubs.acs.org/doi/10.1021/acs.jcim.3c01575

170. Joy, J.; Schaefer, A. J.; Teynor, M. S.$^{\Delta}$; Ess, D. H.* Dynamical Origin of Rebound versus Dissociation Selectivity during Fe-Oxo-Mediated C-H Functionalization Reactions. *J. Am. Chem. Soc.* **2024**, *146*, 2452-2464. https://pubs.acs.org/doi/full/10.1021/jacs.3c09891

169. Stevens, H. P.$^{\Delta}$; Olsen, J.$^{\Delta}$; Kirkland, J. K.; Ess, D. H.* Tolman Electronic Parameter Predictions from a Fast, Accurate, and Robust Machine Learning Model Provide Insight into Phosphine Ligand Electronic Effects. *Organometallics*, **2024**, *43*, 40-47. https://pubs.acs.org/doi/10.1021/acs.organomet.3c00432; ChemRxiv https://chemrxiv.org/engage/chemrxiv/article-details/652438e9bda59ceb9a30feef

168. Chen, S-S.; Meyer, Z.$^{\Delta}$; Jensen, B.$^{\Delta}$; Kraus, A.$^{\Delta}$; Lambert, A.$^{\Delta}$; Ess, D. H.* ReaLigands: A Ligand Library Cultivated from Experiment and Intended for Molecular Computational Catalyst Design. *J. Chem. Inf. Model.* **2023**, *63*, 7412-7422. https://doi.org/10.1021/acs.jcim.3c01310; *ChemRxiv* https://chemrxiv.org/engage/chemrxiv/article-details/64dcf7454a3f7d0c0d45ca3c

167. Luo, J.; Davenport, M. T.; Carter, A.$^{\Delta}$; Ess, D. H.*; Liu, T. L. Mechanistic Studies of Ni-Catalyzed Electrochemical Homo-Coupling Reactions of Aryl Halides. *Faraday Discussions*, **2023**, *247*, 132-142. https://doi.org/10.1039/D3FD00069A

166. Davenport, M. T.; Kirkland, J. K.; Ess, D. H.* Dynamic-dependent selectivity in a bisphosphine iron spin crossover C–H insertion/π-coordination reaction. *Chem. Sci.* **2023**, *14*, 9400-9408. https://pubs.rsc.org/en/content/articlehtml/2023/sc/d3sc02078a

165. Kirkland, J. K.; Joy, J.; Small, B. L.; Leseberg, J. A.; Bischof, S. M.; Webster-Gardiner, M. S.; Ess, D. H.* Rate Limiting Spin Crossover and Cp Ligand Involvement During Ir(III) Retro-Hydroformylation Catalysis. *ACS Catal.* **2023**, *13*, 10895-10907. https://pubs.acs.org/doi/10.1021/acscatal.3c01692

164. Behnke, N. E.; Kwon, Y-D.; Davenport, M. T.; Ess, D. H.*; Kürti, L. Directing-Group-Free Arene C(sp^2)–H Amination using Bulky Aminium Radicals and DFT Analysis of Regioselectivity. *J. Org. Chem.* **2023**, *88*, 11847-11864. https://pubs.acs.org/doi/abs/10.1021/acs.joc.3c01127.

163. Kumawat, J.; Macias, I. D.; Ess, D. H.* Dinuclear Influence on the Mechanism, Reactivity, and Selectivity During Rh–Al-Catalyzed Aryl Ether C–O Bond Reduction/Defunctionalization. *Organometallics*, **2023**, *42*, 1890-1899. https://pubs.acs.org/doi/10.1021/acs.organomet.3c00162; *ChemRxiv* https://chemrxiv.org/engage/chemrxiv/article-details/64246671647e3dca99b59ed3

162. Son, J-Y.; Aikonen, S.; Morgan, N.$^{\Delta}$; Harmata, A. S.; Sabatini, J. J.; Ess, D. H.*; Paton, R. S.; Stephenson, C. R. J. Regioselective Rearrangement of Cubanes to Cuneanes: Scope Expansion and Mechanistic Investigations. *J. Am. Chem. Soc.* **2023**, *145*, 16355-16364. https://pubs.acs.org/doi/full/10.1021/jacs.3c03226; *ChemRxiv* https://chemrxiv.org/engage/chemrxiv/article-details/63ac9e5fe8047a7720f8a702

161. Luo, J.; Davenport, M. T.; Callister, C.; Minteer, S. D.; Ess, D. H.*; Liu, T. L. Understanding Formation and Roles of Ni^{II} Aryl Amido and Ni^{III} Aryl Amido Intermediates in Ni-Catalyzed Electrochemical Aryl Amination Reactions. *J. Am. Chem. Soc.* **2023**, *145*, 16130-16141. https://pubs.acs.org/doi/10.1021/jacs.3c04610; *ChemRxiv* https://doi.org/10.26434/chemrxiv-2022-bpzwt

160. Gunsalus, N.; Koppaka, A.; Chen, S.-S.; Park, S. H. Hashiguchi, B. G.; Ess, D. H.*; Periana, R. A. Reactivity and Mechanisms of Methane, Ethane, and Benzene C-H Amination with an Iodine(III) Bistriflimide Complex. *Organometallics,* **2023**, *42*, 1505-1512. https://pubs.acs.org/doi/10.1021/acs.organomet.3c00122

159. Yang, B.; Mendez-Arroyo, J.; May, C.; Yao, J.; Ess, D. H.* Transition-State Analysis Reveals Unexpected Coordination-Specific Reactivity that Drives Alkene Dimerization by Sulfated Metal–Organic Frameworks. *J. Phys. Chem. C* **2023** *127*, 8539-8546. https://pubs.acs.org/doi/10.1021/acs.jpcc.3c01031; *ChemRxiv* https://doi.org/10.26434/chemrxiv-2022-pv5zx

158. Chen, S.; Rossberg, J.[Δ]; Brown, J.[Δ]; Reed, G.[Δ]; Todd, N.[Δ]; Yu, A.; Fleming, S. A.; Ess, D. H.* Interactive Organic Reaction Trajectory Animation iPhone Application (iORA) and Web Site (webORA). *J. Chem. Ed.* **2023**, *100*, 1659-1663. https://pubs.acs.org/doi/full/10.1021/acs.jchemed.2c00983

157. Joy, J.; Ess, D. H.* Direct Dynamics Trajectories Demonstrate Dynamic Matching and Nonstatistical Radical Pair Intermediates during Fe-Oxo-Mediated C−H Functionalization Reactions. *J. Am. Chem. Soc.* **2023**, *145*, 7628-7637. https://pubs.acs.org/doi/10.1021/jacs.3c01196

156. Maley, S. M.; Lief, G. R.; Buck, R. M.; Sydora, O. L.; Yang, Q.; Bischof, S. M.; Ess, D. H.* Density functional theory and CCSD(T) Evaluation of Ionization Potentials, Redox Potentials, and Bond Energies Related to Zirconocene Polymerization Catalysts. *J. Comput. Chem.* **2023**, *44*, 506-515. https://doi.org/10.1002/jcc.26890

155. Singh, J.; Nelson, T. J.; Mansfield, S. A.; Nickel, G. A.; Cai, Y.; Jones, D. D.; Small, J. E.; Ess, D. H.; Castle, S. L. Microwave- and Thermally Promoted Iminyl Radical Cyclizations: A Versatile Method for the Synthesis of Functionalized Pyrrolines. *J. Org. Chem.* **2022**, *87*, 16250-16262. https://doi.org/10.1021/acs.joc.2c01806

154. Yang, B.; Hawley, D.[Δ]; Yao, J.; May, C.; Mendez-Arroyo, J. E.; Ess, D. H.* "Demonstration of High-Throughput Building Block and Composition Analysis of Metal-Organic Frameworks" *J. Chem. Inf. Model.* **2022**, *62*, 4672-4679. https://doi.org/10.1021/acs.jcim.2c00937

153. Koppaka, A.; Kirkland, J. T.; Periana, R. A.; Ess, D. H.* Experimental Demonstration and Density Functional Theory Mechanistic Analysis of Arene C–H Bond Oxidation and Product Protection by Osmium Tetroxide in a Strongly Basic/Nucleophilic Solvent. *J. Org. Chem.* **2022**, *87*, 13573-13582. https://doi.org/10.1021/acs.joc.2c01159

152. Ess, D. H.*; Jelfs, K. E.; Kulik, H. J. Chemical design by artificial intelligence. *J. Chem. Phys.* **2022**, *157*, 120401. https://doi.org/10.1063/5.0123281

151. Kong, F.; Chen, S.; Chen, J.; Liu, C.; Zhu, W.; Dickie, D. A.; Ess, D. H.*; Zhang, S.; Gunnoe, T. B. Cu(II) Carboxylate Arene C–H Functionalization: Tuning for Non-Radical Pathways. *Sci. Adv.* **2022**, *8*, eadd 1594. DOI: 10.1126/sciadv.add1594

150. Melville, J.[Δ]; Hargis, C.[Δ]; Davenport, M. T.; Hamilton, R. S.[Δ]; Ess, D. H.* Machine Learning Analysis of Dynamic-Dependent Bond Formation in Trajectories with Consecutive Transition States. *J. Phys. Org. Chem.* **2022**, 35, e4405. https://doi.org/10.1002/poc.4405

149. Kattamuri, P. V.; Zhao, J.; Das, T. K.; Siitonen, J. H.; Morgan, N.[Δ]; Ess, D. H.* Kürti, L. *Aza*-Quasi-Favorskii Reaction: Construction of Highly Substituted Aziridines through a Concerted Multibond Rearrangement Process. *J. Am. Chem. Soc*. **2022**, *144*, 10943-10949. https://doi.org/10.1021/jacs.2c03805

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

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