

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

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

- *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)
- *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)

- *Chevron Phillips Chemical Co.*, “Design of Homogeneous Alpha Olefin Catalysts” (PI, 2014-2024)
- *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
- *National Institutes of Health, NIGMS*, “Asymmetric N-H/N-alkyl olefin aziridinations and ring-opening transformations” 1R35GM136373-01 (subcontract, 2020-2025)

COMPLETED AWARDS

- *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 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.
- **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

- >700 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*”. Established in 2018 the goal of this program is to provide a pathway to graduate school. Each year this site hosts 10 visiting undergraduate students and two high school teachers (RET).

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 of annual “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. 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 (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) Comp. Chemist, Nanotech (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) Joeng (Nov. 2023-present)

Sanaz Mohammadzadeh (Jan. 2023-present)

Michael Davenport (June 2020-present)

Dr. Joshua Wheeler, Ph.D. (June 2018-July 2023) *Postdoc in Sweden*

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:

Artem Marchenko, M.S. (Jan. 2022-Dec. 2023) Jointly advised with David Michaelis

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 = 47; i10-index = 109
- Total publications = 171
- Total issued US patents = 10

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 Hydroisindole 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 B1).

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 B1. 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 B1. Issued 11/22/2022.

5. Bischof, S. M.; Sydora, O. L.; Kilgore, U. J.; Ess, D. H.; Kwon, D-H. Chromium Phosphinyl Hydroisindole Amidine Complexes for Tetramerization of Ethylene. (with Chevron Phillips Chem. Co. LP). US 11,492,305 B1. 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 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.

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; ^Δ = undergraduate co-author from my lab)

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**, ASAP. <https://pubs.acs.org/doi/10.1021/acs.jcim.3c01575>
170. Joy, J.; Schaefer, A. J.; Teynor, M. S.; 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.; Olsen, J.; 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. ChemRxiv <https://chemrxiv.org/engage/chemrxiv/article-details/652438e9bda59ceb9a30feef>
168. Chen, S-S.; Meyer, Z.^Δ; Jensen, B.^Δ; Kraus, A.^Δ; Lambert, A.^Δ; 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.^Δ; 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(sp²)-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.^Δ; 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.; Minter, 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-bpzwz>
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](https://doi.org/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 C₆ 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.[△]; 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.[△]; Scott, W.[△]; 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.[△]; 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.[△]; Steagall, R.[△]; Nielson, T.[△]; 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.[△]; 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**, *143*, 8367-8374. <https://pubs.acs.org/doi/10.1021/jacs.1c01709>
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