

DANIEL H. ESS

Associate 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 EXPERIENCE

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

Associate Professor Brigham Young University, Provo Utah (9/16-8/20)

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. Catalysis Advisor: Roy A. Periana
California Institute of Technology (10/07-10/09)
Advisor: William A. Goddard, III

CURRENT RESEARCH AREAS

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

CURRENT EXTERNAL AWARDS (Total for all awards = \$2,489,663)

- *National Science Foundation*, “Dynamical Organometallic Mechanisms” CHE-1952420 (PI, 2020-2023)
- *Chevron Phillips Chemical Co.*, “Design of Homogeneous Alpha Olefin Catalysts” (PI, 2014-2020)
- *Phillips 66*, (PI, 2019-2020)
- *National Science Foundation*, “Theory and Design of Transition-Metal Heterodinuclear and Homodinuclear Catalytic Reactions” CHE-1764194 (PI, 2018-2021)
- *National Science Foundation*, “Chemistry and Biochemistry REU Site to Prepare Students for Graduate School and an Industrial Career” CHE-1757627 (PI, 2018-2021)
- *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 “Modeling and Design of Main-Group Metal Catalyzed Alkane C-H Functionalization Reactions” (PI, 2020-2023) DE-SC0018329

- *National Institutes of Health, NIGMS*, “Asymmetric N-H/N-alkyl olefin aziridinations and ring-opening transformations” 1R35GM136373- 01 (subcontract, 2020-2025)

COMPLETED EXTERNAL AWARDS

- *National Institutes of Health, NIGMS*, “Asymmetric N-H/N-alkyl olefin aziridinations and ring-opening transformations” 1R01GM114609-01 (subcontract, 2015-2019)
- *Utah State, 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

- MECPro: Efficient Python program to locate minimum energy crossing points for organometallic reactions (<http://www.chem.byu.edu/faculty/daniel-h-ess/mecp-software-download/>).
- DynSuite: C++ quasiclassical direct dynamics program.

CHEMISTRY CAMPS

- Creator and co-director of BYU Chem Camp for children ages 9-12 (<https://chemcamp.byu.edu/9-12>) 240 children from 2016-present.
- Creator and co-director of BYU BioChem Camp for youth ages 13-14. (<https://chemcamp.byu.edu/13-14>) 25 youth from 2017-present.
- Creator of Chem 397R course, Mentored Service and Outreach. *This course is used to train BYU undergraduate students as counselors to teach children and youth science.*

SUMMER UNDERGRADUATE AND HIGH SCHOOL TEACHER PROGRAMS

- PI and director of the NSF funded Chemistry and Biochemistry Research Experiences for Undergraduates REU program (established 2018, <https://reu.chem.byu.edu/>). This site hosts 10 visiting undergraduate students, and 2 high school teachers (RET).
- Co-director of the Talmage Research Internship program (<https://www.chem.byu.edu/undergraduate-students/undergraduate-research/talmage-summer-research-internship/>).

TEACHING INNOVATION AND RESEARCH

- **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.

EXTERNAL SERVICE HIGHLIGHTS

- Guest editor for *Chemical Reviews* Volume 119 Issue 11 on “Computational Design of Catalysts from Molecules to Materials”.
- Grant panelist and reviewer for the Department of Energy, the National Science Foundation, and the American Chemical Society Petroleum Research Foundation.

- Reviewed >300 manuscripts from *Science*, *American Chemical Society* journals, *Royal Society of Chemistry* journals, *Elsevier* journals, and *Wiley* journals.
- Cofounder of annual Utah Inorganometallic Conference (2014-2019).

BYU AWARDS

- Karl G. Maeser Research and Creative Arts Award (2019-2020)
- Richard Roskelly Teaching and Learning Fellowship (2017-2018)
- BYU Young Scholar Award (2015)
- BYU College of Physical and Mathematical Sciences Young Scholar Award (2014)

PATENTS

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

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

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

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

BYU PUBLICATIONS (h-index = 37, i10-index = 79; Google Scholar for all publications on 6/23/19)

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

128. Smith, J. D.; Durrant, G.; Ess, D. H.; Gelfand, B. S.; Piers, W. E. “H/D Exchange Under Mild Conditions in Arenes and Unactivated Alkanes with C₆D₆ and D₂O Using Rigid, Electron-rich Iridium PCP Pincer Complexes” *Chem. Sci.* **2020**, <https://doi.org/10.1039/D0SC02694H>

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**, ASAP. <https://doi.org/10.1002/adsc.202000483>

126. Rollins, N.^Δ; Pugh, S. L.^Δ; Maley, S. M.; Grant, B. O.^Δ; Hamilton, S. R.^Δ; Teynor, M. S.^Δ; Carlsen, R.; Jenkins, J. R.^Δ; Ess, D. H.* “Machine Learning Analysis of Direct Dynamics Trajectory Outcomes for Thermal Deazetization of 2,3-Diazabicyclo[2.2.1]hept-2-ene” *J. Phys. Chem. A* **2020**, *124*, 4813-4826. <https://doi.org/10.1021/acs.jpca.9b10410>

125. Wheeler, J.; Carlsen, R.; Ess, D. H.* Mechanistic Molecular Motion of Transition-Metal Mediated β-Hydrogen Transfer: Quasiclassical Trajectories Reveal Dynamically Ballistic, Dynamically Unrelaxed,

Two Step, and Concerted Mechanisms” *Dalton Trans.* **2020**, *49*, 7747-7757.
<https://doi.org/10.1039/D0DT01687J>

124. Gunsalus, N.; Koppaka, A.; Hashiguchi, B.; Konnick, M.; Park, S. H.; Ess, D. H.; Periana, R. “S_N2 and E2 Branching of Main-Group Metal Alkyl Intermediate in Alkane CH Oxidation: A Mechanistic Investigation using Isotopically Labelled Main-Group Metal Alkyls” Submitted. *Organometallics*, **2020**, *39*, 1907-1916. <https://doi.org/10.1021/acs.organomet.0c00120>

123. Avval, T. G.; Hodges, G. T.; Wheeler, J.; Ess, D. H.; Bahr, S.; Dietrich, P.; Meyer, M.; Thißen, A.; Linford, M. R. “Polyethylene terephthalate by near-ambient pressure XPS” *Surface Science Spectra*, **2020**, *27*, 014006. <https://doi.org/10.1116/1.5129466>

122. Teynor, M. S.^Δ; Carlsen, R.; Ess, D. H.* “Relationship Between Energy Landscape Shape and Dynamics Trajectory Outcomes for Methane C-H Activation by Cationic Cp*(PMe₃)Ir/Rh/Co(CH₃)” *Organometallics*, **2020**, *39*, 1393-1403. <https://doi.org/10.1021/acs.organomet.0c00108>

121. Macaulay, C. P.; Samolia, M.; Ferguson, M. J.; Sydora, O. L.; Ess, D. H.*; Stradiotto, M.; Turculet, L. “Synthetic Investigations of Low-Coordinate (N-Phosphino-amidinate) Nickel Chemistry: Agostic Alkyl Complexes and Benzene Insertion into Ni-H” *Dalton Trans.* **2020**, *49*, 4811-4816.
<https://doi.org/10.1039/D0DT00527D>

120. Cheng, Q-Q.; Zhou, Z.; Jiang, H.; Siitonen, J. H.; Ess, D. H.; Zhang, X.; Kürti, L. “Organocatalytic nitrogen transfer to unactivated olefins via transient oxaziridines” *Nat. Cat.* **2020**, *3*, 386–392.
<https://doi.org/10.1038/s41929-020-0430-4>

119. Johnson, B. I.; Avval, T. G.; Wheeler, J. J.; Anderson, H. C.; Diwan, A.; Stowers, K. J.; Ess, D. H.; Linford, M. R. “Semiempirical Peak Fitting Guided by Ab Initio Calculations of X-ray Photoelectron Spectroscopy Narrow Scans of Chemisorbed, Fluorinated Silanes” *Langmuir*, **2020**, *36*, 1878-1886.
<https://doi.org/10.1021/acs.langmuir.9b03136>

118. King, C. R.; Holdaway, A.^Δ; Durrant, G.^Δ; Wheeler, J.; Suaava, L.; Konnick, M. M.; Periana, R. A.; Ess, D. H.* “Supermetal: SbF₅-Mediated Methane Oxidation Occurs by C-H Activation and Isobutane Oxidation Occurs by Hydride Transfer” *Dalton Trans.* **2019**, *48*, 17029-17036.
<https://doi.org/10.1039/C9DT03564H>

117. Aoki, Y.; Bauer, M.; Braun, T.; Cadge, J. Davies, D.; Durand, D.; Eisenstein, O.; Ess, D.; Fairlamb, I.; Fey, N.; Gallarati, S.; George, M.; Greaves, M.; Halse, M.; Hamilton, A.; Harvey, J.; Haynes, A.; Hintermair, U.; Hulme, A.; Ishii, Y.; Jakoobi, M.; Jensen, V. R.; Kennepohl, P.; Kuwata, S.; Lei, A.; Lloyd-Jones, G.; Love, J.; Lovelock, K.; Lynam, J.; Macgregor, S.; Marder, T.; Meijer, E. J.; Morgan, P.; Morris, R.; Mwansa, J.; Nelson, D.; Odom, A.; Perutz, R.; Reiher, M.; Renny, J.; Roithová, J.; Schafer, L.; Schilter, D.; Scott, S.; Slattery, J.; Walton, J.; Wilden, J.; Wong, C.-Y.; Yaman, T. “Physical methods for mechanistic understanding: general discussion” *Faraday Discussions*, **2019**, *220*, 144-178.
<https://doi.org/10.1039/C9FD90070E>

116. Bauer, M.; Cadge, J.; Davies, D.; Durand, D.; Eisenstein, O.; Ess, D.; Fey, N.; Gallarati, S.; George, M.; Hamilton, A.; Harvey, J.; Hintermair, U.; Hulme, A.; Ishii, Y.; Jensen, V. R.; Lloyd-Jones, G.; Love, J.; Lynam, J.; Macgregor, S.; Marder, T.; Meijer, E. J.; Morgan, P.; Morris, R.; Mwansa, J.; Odom, A.; Perutz, R.; Reiher, M.; Schafer, L.; Slattery, J.; Young, T. “Computational and theoretical approaches for mechanistic understanding: general discussion” *Faraday Discussions*, **2019**, *220*, 464-488.
<https://doi.org/10.1039/C9FD90073J>

115. Jain, V.; Wheeler, J. J. Ess, D. H.; Noack, S.; Vacogne, C. D.; Schlaad, H.; Bahr, S.; Dietrich, P.; Meyer, M.; Thißen A.; 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*(PMe₃)Ir(CH₃) Methane C-H Activation Mechanism” *Faraday Discussions*, **2019**, 220, 414-424. <https://doi.org/10.1039/C9FD00035F>
113. Ess, D. H.*; Gagliardi, L.; Hammes-Schiffer, S. “Introduction: Computational Design of Catalysts from Molecules to Materials” *Chem. Rev.* **2019**, 119, 6507-6508. <https://doi.org/10.1021/acs.chemrev.9b00296>
112. Gunsalus, N. J.; Park, S. H.; Hashiguchi, B. G.; Koppaka, A.; Smith, S. J.; Ess, D. H.*; Periana, R. A. “Selective N Functionalization of Methane and Ethane to Aminated Derivatives by Main-Group-Directed C-H Activation” *Organometallics* **2019**, 38, 2319-2322. <https://doi.org/10.1021/acs.organomet.9b00246>
111. Ahn, S.; Hong, M.; Sundararajan, M.; Ess, D. H.*; Baik, M-H. “Design and Optimization of Catalysts Based on Mechanistic Insights Derived from Quantum Chemical Reaction Modeling” *Chem. Rev.* **2019**, 119, 6509-6560. <https://doi.org/10.1021/acs.chemrev.9b00073>
110. Kattamuri, P.; Bhakta, U.; Siriwongsup, S.; Kwon, D-H.; Alemany, L.; Yousefuddin, M.; Ess, D. H.; Kürti, L. “Synthesis of Structurally Diverse 3-, 4-, 5- and 6-Membered Heterocycles from Diisopropyl Iminomalonates and Soft C-Nucleophiles” *J. Org. Chem.* **2019**, 84, 7066-7099. <https://doi.org/10.1021/acs.joc.9b00681>
109. Carlsen, R.; Jenkins, J. R.^Δ; Chuang, J.^Δ; Pugh, S. L.^Δ; Ess, D. H.* “Paddle Ball Dynamics During Rh-Methyl to Rh-Methane σ -Complex Reductive Elimination” *Organometallics* **2019**, 38, 2280-2287. <https://doi.org/10.1021/acs.organomet.8b00936> Cover of Issue 10: <https://pubs.acs.org/toc/orgnd7/38/10>.
108. Cloutier, J-P.; Rechinat, L.; Canac, Y.; Ess, D. H.*; Zargarian, D. “C-O and C-N Functionalization of Cationic, NCN-Type Pincer Complexes of Trivalent Nickel: Mechanism, Selectivity, and Kinetic Isotope Effect” *Inorg. Chem.* **2019**, 58, 3861-3874. <https://doi.org/10.1021/acs.inorgchem.8b03489>
107. Zhang, Y.; Karunananda, M.; Williams, W.^Δ; Clark, K.; Mankad, N.; Ess, D. H.* “Dynamically Bifurcating Hydride Transfer Mechanism and Origin of Inverse Kinetic Isotope Effect for Heterodinuclear AgRu-Catalyzed Alkyne Semi-Hydrogenation” *ACS Catal.* **2019**, 9, 2657-2663. <https://doi.org/10.1021/acscatal.8b04130>
106. Koppaka, A.; Park, S. H.; Hashiguchi, B. G.; Gunsalus, N. J.; King, C. R.; Konnick, M. M.; Ess, D. H.*; Periana, R. A. “Selective C-H Functionalization of Methane and Ethane by a Molecular Sb(V) Complex” *Angew. Chem. Int. Ed.* **2019**, 58, 2241-2245. <https://doi.org/10.1002/anie.201809159>
105. Kwon, D-H.; Small, B.; Sydroa, O. L.; Bischof, S. M.; Ess, D. H.* “The Challenge of Using Practical DFT to Model Fe Pendant Donor Diimine Catalyzed Ethylene Oligomerization” *J. Phys. Chem. B* **2019**, 123, 3727-3739. <https://doi.org/10.1021/acs.jpcc.9b00129>
104. Ess, D. H.* “Rapid Enantioselective Catalyst Optimization” *Nature Catalysis* **2019**, 2, 8-9. <https://doi.org/10.1038/s41929-018-0216-0>

103. Cardon, J. M.; Coombs, J. C.; Ess, D. H. Castle, S. L. “Insights into base-free OsO₄-catalyzed aminohydroxylations employing chiral ligands” *Tetrahedron* **2019**, *75*, 945-948.
102. Behnke, N.; Kielawa, R.; Kwon, D-H.; Ess, D. H.; Kürti, L. “Direct Primary Amination of Alkylmetals with NH-Oxaziridine” *Org. Lett.* **2018**, *20*, 8064-8068.
101. Coombs, J.^Δ; Perry, D.; Kwon, D-H.; Thomas, C. M.; Ess, D. H.* “Why Two Metals Are Better Than One for Cobalt Phosphinoamide Catalyzed Kumada Coupling” *Organometallics* **2018**, *37*, 4195-4203.
100. Macaulay, C. M.; Gustafson, S. J.; Fuller, J. T., III; Kwon, D-H.; Ogawa, T.; Ferguson, M. J.; McDonald, R.; Lumsden, M. D.; Bischof, S. M.; Sydora, O. L.; Ess, D. H.*; Stradiotto, M.; Turculet L. “Alkene Isomerization-Hydroboration Catalyzed by First-Row Transition Metal (Mn, Fe, Co, and Ni) *N*-Phosphinoamidinate Complexes: Origin of Reactivity and Selectivity” *ACS Catal.* **2018**, *8*, 9907-9925.
99. Lovato, K.; Guo, L.; Xu, Q-L.; Liu, F.; Yousufuddin, M.; Ess, D. H.*; Kürti, L.; Gao, H. “Transition Metal-Free Direct Dehydrogenative Arylation of Activated C(sp³)-H Bonds: Synthetic Ambit and DFT Reactivity Predictions” *Chem. Sci.* **2018**, *9*, 7992-7999.
98. Carlsen, R.; Wohlgemuth, N.^Δ; Carlson, L.^Δ; Ess, D. H.* “Dynamical Mechanism May Avoid High-Oxidation State Ir(V)-H Intermediate and Coordination Complex in Alkane and Arene C-H Activation by Cationic Ir(III) Phosphine” *J. Am. Chem. Soc.* **2018**, *140*, 11039-11045.
97. King, C. R.; Rollins, N.^Δ; Holdaway, A.^Δ; Konnick, M. M.; Periana, R. A.; Ess, D. H.* “Electrophilic Impact of High-Oxidation State Main-Group Metal and Ligands on Methane C-H Activation and Functionalization Reactions” *Organometallics*, **2018**, *37*, 3045-3054.
96. Gustafson, S. J.; Konnick, M. M.; Periana, R. A.; Ess, D. H.* “Mechanisms and Reactivity of Tl(III) Main-Group Metal-Alkyl Functionalization in Water” *Organometallics*, **2018**, *37*, 2723-2731.
95. Saavedra, D. I.; Rencher, B. D.; Kwon, D-H.; Smith, S. J.; Ess, D. H.*; Andrus, M. B. “Synthesis and Computational Studies Demonstrate the Utility of an Intramolecular Styryl Diels-Alder Reaction and BHT Assisted [1,3]-shift to Construct Anticancer *dl*-Deoxy podophyllotoxin” *J. Org. Chem.* **2018**, *83*, 2018-2026.
94. Kwon, D-H.; Fuller, J. T. III; Kilgore, U. J.; Sydora, O. L.; Bischof, S. M.; Ess, D. H.* “Computational Transition-State Design Provides Experimentally Verified Cr(P,N) Catalysts for Control of Ethylene Trimerization and Tetramerization” *ACS Catal.* **2018**, *8*, 1138-1142.
93. Kattamuri, P. V.; Yin, J.; Siriwongsup, S.; Kwon, D-H.; Ess, D. H.; Li, Q.; Li, G.; Yousufuddin, M.; Richardson, P. F.; Sutton, S. C.; Kürti, L. “Practical Singly and Doubly electrophilic Aminating Agents: A New, More Sustainable Platform for Carbon–Nitrogen Bond Formation” *J. Am. Chem. Soc.* **2017**, *139*, 11184-11196.
92. Kwon, D-H.; Proctor, M.^Δ; Mendoza, S.^Δ; Uyeda, C.; Ess, D. H.* “Catalytic Dinuclear Nickel Spin Crossover Mechanism and Selectivity for Alkyne Cyclotrimerization” *ACS Catal.* **2017**, *7*, 4796-4804.
91. Gao, H.; Zhou, Z.; Kwon, D-H.; Coombs, J.^Δ; Jones, S.^Δ; Behnke, N. E.; Ess, D. H.*; Kürti, L. “Rapid heteroatom transfer to arylmetals utilizing multifunctional reagent scaffolds” *Nature Chemistry* **2017**, *9*, 681-688.

90. Kelly, C. M.; Fuller, J. T., III; Macaulay, C. M.; McDonald, R.; Ferguson, M. J.; Bischof, S. M.; Sydora, O. L.; Ess, D. H.*; Stradiotto, M.; Turculet, L. "Dehydrogenative B-H/C(sp³)-H Benzylic Borylation within the Coordination Sphere of Platinum(II)" *Angew. Chem. Int. Ed.* **2017**, *56*, 6312-6316.
89. King, C. R.; Gustafson, S. J.; Black, B. R.^Δ; Butler, S. K.^Δ; Konnick, M. K.; Periana, R. A.; Hashiguchi, B. M.; Ess, D. H.* "Arene C-H Functionalization by p-Block Metal Tl(III) Occurs at the Borderline of C-H Activation and Electron Transfer" *Organometallics*, **2017**, *36*, 109-113.
88. Paudyal, M. P.; Adebessin, A. M.; Burt, S. R.; Ess, D. H.; Ma, Z.; Kürti, L.; Falck, J. R. "Dirhodium Catalyzed C-H Arene Amination using Hydroxylamines" *Science* **2016**, *353*, 1144-1147.
87. Fuller, J. T., III; Butler, S.^Δ; Devarajan, D.; Jacobs, A.^Δ; Hashiguchi, B. G.; Konnick, M. M.; Goddard, W. A., III; Gonzales, J.; Periana, R. A.; Ess, D. H.* "Catalytic Mechanism and Efficiency of Methane Oxidation by Hg(II) in Sulfuric Acid and Comparison to Radical Initiated Conditions" *ACS Catal.* **2016**, *6*, 4312-4322.
86. Carlsen, R.; Ess, D. H.* "Allylic amination reactivity of Ni, Pd, and Pt Heterobimetallic and Monometallic Complexes" *Dalton Trans.* **2016**, *45*, 9835-9840.
85. Xu, Q-L.; Keene, C.; Yousufuddin, M.; Ess, D. H.; Kürti, L. "Practical Organocatalytic Synthesis of Functionalized Non-C₂-Symmetrical Atropisomeric Biaryls" *Angew. Chem. Int. Ed.* **2016**, *128*, 576-581.
84. King, C. R.; Gustafson, S. J.; Ess, D. H.* "The Electronics of CH Activation by Energy Decomposition Analysis: From Transition Metals to Main-Group Metals" *Structure and Bonding*, Vol. 167, **2015**, 163-178.
83. Sheng, M.; Jiang, N.; Gustafson, S. You, B.; Ess, D. H.*; Sun, Y. "A nickel complex with a biscarbene pincer-type ligand shows high electrocatalytic reduction of CO₂ over H₂O" *Dalton Trans.* **2015**, *44*, 16247-16250.
82. Kelly, C. M.; Kwon, D-H.; Ferguson, M. J.; Bischof, S. M.; Sydora, O. L.; Ess, D. H.*; Stradiotto, M.; Turculet, L. "Synthesis and Reactivity of a Neutral, Three-Coordinate Platinum(II) Complex Featuring Terminal Amido Ligation" *Angew. Chem. Int. Ed.* **2015**, *127*, 14498-14502.
81. Gustafson, S. J.; Fuller, J. T. III; Devarajan, D.; Snyder, J.; Periana, R. A.; Hashiguchi, B. G.; Konnick, M. M.; Ess, D. H.* "Contrasting Mechanisms and Reactivity of Tl(III), Hg(II), and Co(III) for Alkane C-H Functionalization" *Organometallics* **2015**, *34*, 5485-5495.
80. Fuller J. T.; Harrison, D. J.; Leclerc, M. C.; Baker, R. T.; Ess, D. H.*; Hughes, R. P. "A New Stepwise Mechanism for Formation of a Metallacyclobutane via a Singlet Diradical Intermediate" *Organometallics* **2015**, *34*, 5210-5213.
79. Brosnahan, A. M.; Talbot, A.; McKeown, B. A.; Kalman, S. E.; Gunnoe, T. B.; Ess, D. H.*; Sabat, M. "Phosphine and N-heterocyclic carbene ligands on Pt(II) shift selectivity from ethylene hydrophenylation toward benzene vinylation" *J. Organomet. Chem.* **2015**, *793*, 248-255.
78. Walker, W. K.; Kay, B. M.^Δ; Michaelis, S. A.; Anderson, D. L.; Smith, S. J.; Ess, D. H.*; Michaelis, D. J. "Origin of Fast Catalysis in Allylic Amination Reactions Catalyzed by Pd-Ti Heterobimetallic Complexes" *J. Am. Chem. Soc.* **2015**, *137*, 7371-7378.

77. Zhang, Y.; Roberts, S. P.^Δ; Bergman, R. G.; Ess, D. H.* “Mechanism and Catalytic Impact of Ir-Ta Heterobimetallic and Ir-P Transition Metal/Main Group Interactions on Alkene Hydrogenation” *ACS Catal.* **2015**, *5*, 1840-1849.
76. Devarajan, D.; Gustafson, S. J.; Bickelhaupt, F. M.; Ess, D. H.* “Is There a Need to Discuss Atomic Orbital Overlap When Teaching Hydrogen-Halide Bond Strength and Acidity Trends in Organic Chemistry?” *J. Chem. Ed.* **2015**, *92*, 286-290.
75. Talbot, A.^Δ; Devarajan, D.; Gustafson, S. J.; Fernández, I.; Bickelhaupt, F. M.; Ess, D. H.* “Activation-Strain Analysis Reveals Unexpected Origin of Fast Reactivity in Heteroaromatic Azadiene Inverse-Electron-Demand Diels-Alder Cycloadditions” *J. Org. Chem.* **2015**, *80*, 548-558.
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