

Curriculum Vitae

Name: Deven P. Estes, Jun.-Prof. Dr.
Address: Pfaffenwaldring 55, 70569 Stuttgart
Telephone: (0)711 68564060
E-mail: deven.estes@itc.uni-stuttgart.de
Date of Birth: 17.05.1987 (Chickasha, OK, USA)
Citizenship: USA
Marital Status: Married



Education

Ph.D. Columbia University, Research Director Jack Norton (2014)
M.Phil., Columbia University, Research Director Jack Norton (2013)
M.A., Columbia University, Research Director Jack Norton (2011)
B.S., University of Oklahoma, Research Director Kenneth M. Nicholas (2009)
High School, Cement High School, Cement, OK (2005)

Employment History

Junior Professor (TT - W3), Institute for Technical Chemistry, University of Stuttgart (2019-pres)
Postdoctoral Fellow, MPI for Chemical Energy Conversion, Research Director Walter Leitner (2018-19)
Postdoctoral Fellow, RWTH Aachen, Research Director Walter Leitner (2017-18)
Postdoctoral Fellow, ETH Zürich, Research Director Christophe Copéret (2014-17)

Research Interests

Surface Organometallic Chemistry, Molecular Heterogeneous Catalysis, Mechanistic Chemistry, Reactive Intermediates, Kinetics and Thermodynamics of Catalytic Processes, Technical Chemistry

Fellowships and Awards

Catalysis Science and Technology Emerging Investigator (2021)
Marie Curie ETH Zürich Postdoctoral Fellowship (2015)
Pegram Award for Excellent Doctoral Work, Columbia University (2014)
Miller Teaching Award, Columbia University (2011)
US Department of Energy Office of Science National Graduate Fellowship (2010)
Dick Van der Helm Undergraduate Research Fellowship (2008)

Languages

English (Native)
German (Fluent)

Presentations

Deven P. Estes, Understanding Metal-Support Interactions Using Well-Defined Surface Metal Hydrides Synthesized by Surface Organometallic Chemistry and Molecular Heterogeneous Catalysis, International Symposium on the Relations between Homogeneous and Heterogeneous Catalysis (ISHHC 19), Online (Oslo, Norway), June 29th, 2022.

Deven P. Estes, Transition-Metal Hydrides Immobilized on Metal Oxide Surfaces: Understanding Metal Support Interactions in Heterogeneous CO₂ Hydrogenation Catalysts, Green Chemistry and C1 Value Symposium, Chembio Finland 2022, Helsinki, Finland, June, 8th, 2022.

Deven P. Estes, Interactions between Metal Hydride Complexes and Metal Oxide Surfaces: Effect of Confinement on CO₂ Hydrogenation, CataLysis Symposium, Kassel, DE, May 3rd, 2022.

Deven P. Estes, Andreas Rosen, Walter Leitner, Jürgen Klankermayer, Tailored Catalyst System for the Synthesis of Dimethoxymethane from CO₂ and Molecular Hydrogen, 18th International Symposium on Relations between Homogeneous and Heterogeneous Catalysis, July 23rd, 2018, Sydney, AU

Deven P. Estes, The Effect of Electron-Withdrawing Ligands on Alkyne Metathesis Catalysts: Insights from Solid State NMR, International Symposium on Olefin Metathesis and related reactions (ISOM) XXII, July 11th, 2017, Zürich, CH

Deven P. Estes, G. Siddiqui, F. Allouche, K. V. Kovtunov, O. V. Safonova, A. Trigub, I. V. Koptuyug, C. Copéret, C-H Activations Catalyzed by Transition-Metal Ions Isolated on Metal Oxide Surfaces, Swiss Chemical Society Fall Meeting 2016, September 15th, 2016, Zürich, CH

Deven P. Estes, David C. Grills, Gang Li, Jack R. Norton; Investigation of the Co-H Bond in Solvated Cobaloximes, In *Abstracts of Papers*, Proceedings of the 246th ACS National Meeting and Exposition, Indianapolis, IN, September 8-12th, 2013; American Chemical Society: Washington, DC, 2013

Jack R. Norton, Deven P. Estes, Aaron K. Vannucci, Ariel Hall, Dennis L. Lichtenberger; Acidities and metal-hydrogen bond dissociation energies of (η^5 -C₅R₅)M(CO)₂H (M= Fe, Ru, Os) (R = H, Me), In *Abstracts of Papers*, Proceedings of the 241st ACS National Meeting and Exposition, Anaheim, CA, March 27-31st, 2011; American Chemical Society: Washington, DC, 2011

Publications

27. Yuji Ikeda, Deven P. Estes, Blazej Grabowski, Comprehensive Understanding of H Adsorption on MoO₃ from Systematic Ab Initio Simulations, *J. Phys. Chem. C*, **2022**, 126, 7728. DOI: [10.1021/acs.jpcc.2c01085](https://doi.org/10.1021/acs.jpcc.2c01085)

26. Abdulhamid H. Almidani, Michael Benz, Mario Winkler, Yuji Ikeda, Blazej Grabowski, Joris van Slageren, Deven P. Estes, The reaction of HV(CO)₄dppe with MoO₃: a well-defined model of hydrogen spillover, *Catal. Sci. Technol. Emerging Investigator Series*, **2021**, 11, 7540. DOI: [10.1039/D1CY01374B](https://doi.org/10.1039/D1CY01374B)

25. Carolin Rieg, Daniel Dittmann, Zheng Li, Dr. Robert Lawitzki, Katrin Gugeler, Sarah Maier, Prof. Guido Schmitz, Prof. Johannes Kästner, Prof. Deven P. Estes, Dr. Michael Dybala, Quantitative Distinction between Noble Metals Located in Mesopores from Those on the External Surface, *Chem. Eur. J.*, **2021**, 27, 17012. DOI: <https://doi.org/10.1002/chem.202102076>.

24. Hoang-Huy Nguyen, Zheng Li, Toni Enenkel, Joachim Hildebrand, Matthias Bauer, Michael Dybala, and Deven P. Estes, Probing the Interactions of Immobilized Ruthenium Dihydride Complexes with Metal Oxide Surfaces by MAS NMR: Effects on CO₂ Hydrogenation, *J. Phys. Chem. C*, **2021**, 125, 14627. DOI: [10.1021/acs.jpcc.1c02074](https://doi.org/10.1021/acs.jpcc.1c02074).

23. Sarah Maier, Steve P. Cronin, Manh-Anh Vu Dinh, Zheng Li, Michael Dybala, Michal Nowakowski, Matthias Bauer, Deven P. Estes, Immobilized Platinum Hydride Species as Catalysts for Olefin Isomerizations and Enyne Cycloisomerizations, *Organometallics*, **2021**, 40, 1751. DOI: [10.1021/acs.organomet.1c00216](https://doi.org/10.1021/acs.organomet.1c00216).

22. Carolin Rieg, Daniel Dittmann, Zheng Li, Alan Kurtz, Isabelle Lorenz, Deven P. Estes, Michael Buchmeiser, Michael Dybala, Michael Hunger, Noble metal location in porous supports

determined by reaction with phosphines, *Micropor. Mesopor. Mat.*, **2021**, 310, 110594. DOI: [10.1002/chem.202102076](https://doi.org/10.1002/chem.202102076).

21. Sven Lang, Michael Dyballa, Yvonne Traa, Deven P. Estes, Elias Klemm, Michael Hunger, Direct Proof of Volatile and Adsorbed Hydrocarbons on Solid Catalysts by Complementary NMR Methods, *Chem. Ing. Tech.* **2021**, 93, 1020. DOI: [10.1002/cite.202000128](https://doi.org/10.1002/cite.202000128).

20. Manuel Kirchhof, Katrin Gugeler, Felix Richard Fischer, Michal Nowakowski, Alina Bauer, Sonia Alvarez-Barcia, Karina Abitaev, Marc Schnerle, Yaseen Qawasmi, Wolfgang Frey, Angelika Baro, Deven P. Estes, Thomas Sottmann, Mark R. Ringenberg, Bernd Plietker, Matthias Bauer, Johannes Kästner, and Sabine Laschat, Experimental and Theoretical Study on the Role of Monomeric vs Dimeric Rhodium Oxazolidinone Norbornadiene Complexes in Catalytic Asymmetric 1,2- and 1,4-Additions, *Organometallics*, **2020**, 39, 3131. DOI: [10.1021/acs.organomet.0c00310](https://doi.org/10.1021/acs.organomet.0c00310)

19. Deven P. Estes, Markus Leutsch, Lukas Schubert, Alexis Bordet, Walter Leitner, The Effect of Ligand Electronics on the Reversible Catalytic Hydrogenation of CO₂ to Formic Acid using Ruthenium Polyhydride Complexes: A Thermodynamic and Kinetic Study, *ACS Catal.*, **2020**, 10, 2990. DOI: <https://pubs.acs.org/doi/abs/10.1021/acscatal.0c00404>

18. Scott R. Docherty, Deven P. Estes, Christophe Copéret, Facile Synthesis of Unsymmetrical Trialkoxysilanols: (RO)₂(R'O)SiOH, *Helv. Chim. Acta*, **2018**, e1700298. DOI: <https://onlinelibrary.wiley.com/doi/full/10.1002/hlca.201700298>

17. Deven P. Estes, Christopher P. Gordon, Alexey Fedorov, Wei-Chih Liao, Henrike Ehrhorn, Celine Bittner, Manuel Luca Zier, Dirk Bockfeld, Ka Wing Chan, Odile Eisenstein, Christophe Raynaud, Matthias Tamm, Christophe Copéret, Molecular and Silica-Supported Molybdenum Alkyne Metathesis Catalysts: Influence of Electronics and Dynamics on Activity Revealed by Kinetics, Solid-State NMR, and Chemical Shift Analysis, *J. Am. Chem. Soc.*, **2017**, 139, 17597. DOI: <https://pubs.acs.org/doi/abs/10.1021/jacs.7b09934>

16. Deven P. Estes, Amanda K. Cook, Erwin Lam, Louise Wong, Christophe Copéret, Understanding the Lewis Acidity of Co(II) Sites on a Silica Surface, *Inorg. Chem.* **2017**, 56, 7731. DOI: <https://pubs.acs.org/doi/abs/10.1021/acs.inorgchem.7b00443>

15. Deven P. Estes, Mechanistic Investigations of C–H Activations on Silica-Supported Co (ii) Sites in Catalytic Propane Dehydrogenation, *Chimia*, **2017**, 71, 177. DOI: <https://www.ingentaconnect.com/contentone/scs/chimia/2017/00000071/00000004/art00005>

14. Murielle Delley, Marius Silaghi, Francisco Nuñez-Zarur, Kirill Kovtunov, Oleg Salnikov, Deven P. Estes, Igor Koptuyug, Aleix Comas-Vives, Christophe Copéret, X-H Bond Activation on Cr(III),O Sites (X = R or H) : Key Steps in Dehydrogenation and Hydrogenation Processes, *Organometallics*, **2017**, 36, 234. DOI: <https://pubs.acs.org/doi/abs/10.1021/acs.organomet.6b00744>

13. Deven P. Estes, Georges Siddiqi, Florian Allouche, Kirill V. Kovtunov, Olga V. Safonova, Alexander L. Trigub, Igor V. Koptuyug, Christophe Copéret, C-H activation on Co,O Sites: Isolated Surface Sites versus Molecular Analogues, *J. Am. Chem. Soc.*, **2016**, 138, 14987. DOI: <https://pubs.acs.org/doi/abs/10.1021/jacs.6b08705>

12. Deven P. Estes, Celine Bittner, Óscar Àrias, Martin Casey, Alexey Fedorov, Matthias Tamm, and Christophe Copéret, Alkyne Metathesis at ppm Catalyst Loading, *Angew. Chem. Int. Ed.*, **2016**, 55, 14166. DOI: <https://onlinelibrary.wiley.com/doi/full/10.1002/anie.201605129>
11. Christophe Copéret, Deven P. Estes, Kim Larmier, Keith Searles, Isolated Surface Hydrides: Formation, Structure and Reactivity, Thematic Issue on Metal Hydrides, *Chem. Rev.* **2016**, 116, 8463. DOI: <https://pubs.acs.org/doi/abs/10.1021/acs.chemrev.6b00082>
10. Yue Hu, Anthony P. Shaw, Deven P. Estes, Jack R. Norton; Transition-Metal Hydride Cation Radicals, Thematic Issue on Metal Hydrides, *Chem. Rev.* **2016**, 116, 8427. DOI: <https://pubs.acs.org/doi/abs/10.1021/acs.chemrev.5b00532>
9. Christophe Copéret, Aleix Comas-Vives, Matthew P. Conley, Deven P. Estes, Alexey Fedorov, Victor Mougel, Haruki Nagae, Francisco Núñez-Zarur, Pavel A. Zhizhko; Surface Organometallic and Coordination Chemistry toward Single-Site Heterogeneous Catalysts: Strategies, Methods, Structures, and Activities, *Chem. Rev.* **2016**, 116, 323. DOI: <https://pubs.acs.org/doi/abs/10.1021/acs.chemrev.5b00373>
8. Deven P. Estes, Christophe Copéret; The Role of Proton Transfer in Heterogeneous Transformations of Hydrocarbons, *Chimia*, **2015**, 69, 321. DOI: <https://www.ingentaconnect.com/content/scs/chimia/2015/00000069/00000006/art00003>
7. Deven P. Estes, David C. Grills, Jack R. Norton; The Reaction of Cobaloximes with Hydrogen: Products and Thermodynamics, *J. Am. Chem. Soc.* **2014**, 136, 17362. DOI: <https://pubs.acs.org/doi/abs/10.1021/ja508200g>
6. Gang Li, Deven P. Estes, Jack R. Norton, Serge Rucollo, Aaron Sattler; Dihydrogen Activation by Cobaloximes with Various Axial Ligands, *Inorg. Chem.* **2014**, 53, 10743. DOI: <https://pubs.acs.org/doi/abs/10.1021/ic501975r>
5. Jay C. Poret, Anthony P. Shaw, Christopher M. Csernica, Karl D. Oyler, Deven P. Estes, Development and Performance of the W/Sb₂O₃/KIO₄/ Lubricant Pyrotechnic Delay in the US Army Hand-Held Signal, *Prop., Expl., Pyrotech.* **2013**, 38, 35. DOI: <https://onlinelibrary.wiley.com/doi/full/10.1002/prop.201200109>
4. Deven P. Estes, Jack R. Norton, Steffen Jockusch, Wesley Sattler; Mechanisms by which Alkynes React with CpCr(CO)₃H. Application to Radical Cyclization, *J. Am. Chem. Soc.* **2012**, 134, 15512. DOI: <https://pubs.acs.org/doi/abs/10.1021/ja306120n>
3. Gang Li, Arthur Han, Mary E. Pulling, Deven P. Estes, Jack R. Norton; Evidence for Formation of a Co-H bond in (H₂O)₂Co(dmgbF₂)₂ under H₂: Application to Radical Cyclization, *J. Am. Chem. Soc.* **2012**, 134, 14662. DOI: <https://pubs.acs.org/doi/abs/10.1021/ja306037w>
2. Deven P. Estes, Aaron K. Vannucci, Ariel R. Hall, Dennis L. Lichtenberger, Jack R. Norton; Thermodynamics of the Metal – Hydrogen Bond in (η⁵-C₅H₅)M(CO)₂H (M = Fe, Ru, Os), *Organometallics* **2011**, 30, 3444. DOI: <https://pubs.acs.org/doi/abs/10.1021/om2001519>
1. Masaomi Matsumoto, Deven Estes, Kenneth M. Nicholas; Evolution of Metal Complex-Catalysts by Dynamic Templating with Transition State Analogs; *Eur. J. Inorg. Chem.* **2010**, 12, 1847. DOI: <https://onlinelibrary.wiley.com/doi/full/10.1002/ejic.201000129>