Joseph Montoya

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Education

2015 Ph.D. Chemical Engineering, **Stanford University**, Stanford, CA
Thesis: "Theoretical electrocatalysis for renewable fuels and chemicals"

2014 M.S. Chemical Engineering, **Stanford University**, Stanford, CA

2010 B.S. Chemical Engineering, **University of South Carolina**, Columbia, SC
2010 B.S. Mathematics, **University of South Carolina**, Columbia, SC
2010 Certificate, Piano Performance, **University of South Carolina**, Columbia SC

Professional History

2015-Current | Postdoctoral Researcher, **Lawrence Berkeley National Laboratory**
Advisor: Kristin Persson, Energy Environental Technologies Division
Part of the core development team for the Materials Project. Projects include performing high-throughput calculations of elastic tensors, developing workflows for surface science, refining approaches to electrochemical stability analysis, and determining trends in complex oxide reactivity for solar water splitting and CO_2 reduction

2010-2015 | Graduate Student Researcher, **Stanford University**
Advisor: Jens Nørskov, Dept. of Chemical Engineering
Performed DFT simulations of the electrocatalysis of nitrogen electroreduction, total water splitting on perovskite oxides, and C-C coupling in CO_2 electroreduction. Constructed linear scaling relations to identify trends and structure sensitivity of various catalytic surfaces. Used and developed electrochemical kinetics in CatMAP software to model steady-state turnover and selectivity. Created tools for managing data corresponding to over 5000 bulk compounds, 500 surfaces, and 10000 adsorbate configurations.

2006-2010 | Undergraduate Researcher, **University of South Carolina**
Advisors: John Monnier, Chris Williams, Dept. of Chemical Engineering
Conducted experimental synthesis and characterization of bimetallic catalysts for the selective hydrogenation of acetylene and epoxybutene. Used electroless deposition (ED) technique to prepare [Cu,Ag,Au][Pd,Pt]/SiO_2 bimetallic catalysts. Characterized catalyst surface area and activity.

2008 | IREU, **King Mongkut University of Technology, Thonburi, Thailand**
Advisors: Preecha Termsuksawad, Dept. of Materials Science
Studied extraction of Ni-Co alloys from spent nickel metal-hydride (Ni-MH) batteries via electrochemical characterization with cyclic voltammetry (CV) and chronoamperometry.

Selected Awards and Honors

2014 Outstanding Chemical Engineering TA Award, **Stanford University**
2013 Richard J. Kokes Award, **North American Catalysis Society**
2010 Graduate Research Fellowship, **National Science Foundation**
2010 Finalist, **Rhodes Scholarship**
2008 **Barry M. Goldwater Scholarship**

Publications

[1] Cave, E. R., **Montoya, J. H.**, Kuhl, K. P., Abram, D. N., Hatsukade, T., Shi, C., Hahn, C., Nørskov, J. K., Jaramillo, T. F., "Electrochemical CO ‹sub›2‹/sub› reduction on Au surfaces: mechanistic aspects regarding the formation of major and minor products". *Phys. Chem. Chem. Phys.* 19.24 (2017), pp. 15856–15863.

[2] Dagdelen, J., **Montoya, J.**, Jong, M., Persson, K., "Computational prediction of new auxetic materials". *Nature Communications* 8.1 (Dec. 2017), p. 323.

[3] Mathew, K., **Montoya, J. H.**, Faghaninia, A., Dwarakanath, S., Aykol, M., Tang, H., Chu, I., Smidt, T., Bocklund, B., Horton, M., Dagdelen, J., Wood, B., Liu, Z. K., Neaton, J., Ong, S. P., Persson, K., Jain, A., "Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows". *Computational Materials Science* 139 (Nov. 2017), pp. 140–152.

[4] **Montoya, J. H.**, Persson, K. A., "A high-throughput framework for determining adsorption energies on solid surfaces". *npj Computational Materials* 3.1 (2017), p. 14.

[5] **Montoya, J. H.**, Seitz, L. C., Chakthranont, P., Vojvodic, A., Jaramillo, T. F., Nørskov, J. K., "Materials for solar fuels and chemicals". *Nature Materials* 16 (2017).

[6] Bertheussen, E., Verdaguer-Casadevall, A., Ravasio, D., **Montoya, J. H.**, Trimarco, D. B., Roy, C., Meier, S., Wendland, J., Nørskov, J. K., Stephens, I. E. L., Chorkendorff, I., "Acetaldehyde as an Intermediate in the Electroreduction of Carbon Monoxide to Ethanol on Oxide-Derived Copper". *Angewandte Chemie* 128.4 (Jan. 2016), pp. 1472–1476.

[7] Latimer, A. A., Kulkarni, A. R., Aljama, H., **Montoya, J. H.**, Yoo, J. S., Tsai, C., Abild-Pedersen, F., Studt, F., Nørskov, J. K., "Understanding trends in C–H bond activation in heterogeneous catalysis". *Nature Materials* (Oct. 2016).

[8] Sandberg, R. B., **Montoya, J. H.**, Chan, K., Nørskov, J. K., "CO-CO coupling on Cu facets: Coverage, strain and field effects". *Surface Science* 654 (2016), pp. 56–62.

[9] Seitz, L. C., Dickens, C. F., Nishio, K., Hikita, Y., **Montoya, J.**, Doyle, A., Kirk, C., Vojvodic, A., Hwang, H. Y., Norskov, J. K., Jaramillo, T. F., "A highly active and stable IrO x /SrIrO 3 catalyst for the oxygen evolution reaction". *Science* 353.6303 (2016), pp. 1011–1014.

[10] Tsai, C., Lee, K., Yoo, J. S., Liu, X., Aljama, H., Chen, L. D., Dickens, C. F., Geisler, T. S., Guido, C. J., Joseph, T. M., Kirk, C. S., Latimer, A. A., Loong, B., McCarty, R. J., **Montoya, J. H.**, Power, L., Singh, A. R., Willis, J. J., Winterkorn, M. M., Yuan, M., Zhao, Z.-J., Wilcox, J., Nørskov, J. K., "Direct Water Decomposition on Transition Metal Surfaces: Structural Dependence and Catalytic Screening". *Catalysis Letters* 146.4 (Feb. 2016), pp. 718–724.

[11] Doyle, A. D., **Montoya, J. H.**, Vojvodic, A., "Improving Oxygen Electrochemistry through Nanoscopic Confinement". *ChemCatChem* 7.5 (Mar. 2015), pp. 738–742.

[12] **Montoya, J. H.**, Shi, C., Chan, K., Nørskov, J. K., "Theoretical Insights into a CO Dimerization Mechanism in CO2 Electroreduction". *The Journal of Physical Chemistry Letters* 6.11 (2015), pp. 2032–2037.

[13] **Montoya, J. H.**, Tsai, C., Vojvodic, A., Nørskov, J. K., "The Challenge of Electrochemical Ammonia Synthesis: A New Perspective on the Role of Nitrogen Scaling Relations." *ChemSusChem* 8.13 (2015), pp. 2180–6.

[14] Wang, Y., **Montoya, J. H.**, Tsai, C., Ahlquist, M. S. G., Nørskov, J. K., Studt, F., "Scaling Relationships for Binding Energies of Transition Metal Complexes". *Catalysis Letters* (Dec. 2015).

[15] **Montoya, J. H.**, Garcia-Mota, M., Nørskov, J. K., Vojvodic, A., "Theoretical evaluation of the surface electrochemistry of perovskites with promising photon absorption properties for solar water splitting". *Phys. Chem. Chem. Phys.* (2014), pp. 2634–2640.

[16] Hansen, H. A., **Montoya, J. H.**, Zhang, Y. J., Shi, C., Peterson, A. a., Nørskov, J. K., "Electroreduction of methanediol on copper". *Catalysis Letters* 143.7 (2013), pp. 631–635.

[17] **Montoya, J. H.**, Peterson, A. a., Nørskov, J. K., "Insights into C-C Coupling in CO2 Electroreduction on Copper Electrodes". *ChemCatChem* 5.3 (2013), pp. 737–742.

[18] Schaal, M. T., Metcalf, A. Y., **Montoya, J. H.**, Wilkinson, J. P., Stork, C. C., Williams, C. T., Monnier, J. R., "Hydrogenation of 3,4-epoxy-1-butene over Cu–Pd/SiO2 catalysts prepared by electroless deposition". *Catalysis Today* 123.1-4 (2007), pp. 142–150.

Forthcoming Publications

[1] **Montoya, J. H.**, Doyle, A. D., Vojvodic, A., Nørskov, J. K., "Trends in adsorption of electrocatalytic water splitting intermediates on cubic ABO3 oxides". *Submitted* (2017).

[2] **Montoya, J.**, Winter, I. S., Dwaraknath, S., Dagdalen, J., Mathew, K., Jong, M., Asta, M., Chrzan, D., Persson, K. A., "New methodologies and applications of elastic tensors from density functional theory". *In preparation* (2017).

[3] Singh, A. R., **Montoya, J. H.**, Rohr, B., Tsai, C., Vojvodic, A., Nørskov, J. K., "Computational Design of Active Site Structures with Improved Transition-State Scaling for Ammonia Synthesis". *Submitted* (2017).

[4] Singh, A. K., Zhou, L., Shinde, A., Suram, S. K., **Montoya, J. H.**, Gregoire, J. M., Persson, K. A., "Electrochemical stability of metastable materials". *Submitted* (2017).

Selected Recent and Upcoming Talks

November 2017
- A High-Throughput Computational Screening Approach for Solar Fuels Photoelectrocatalysis
- New Milestones and Challenges to High-Throughput Computation of Elastic Properties on the Materials Project
- Climbing the Volcano: Active-Site Engineering at the Atomic Scale

AIChE Annual Meeting, Minneapolis, MN

September 2017
- The Materials Project: Challenges and Opportunities in High-throughput computational Materials Science

E-CAM Industry Workshop, "From Atom to Material", Cambridge, UK

August 2017
- Towards a solar fuels future: Theoretical metrics for photoelectrocatalyst screening
- High-throughput workflows for determining adsorption energies on solid surfaces

ACS Fall Meeting, Washington, DC

June 2017
- The Materials Project: Challenges and Opportunities in High-throughput computational Materials Science

ECS Annual Meeting, New Orleans, LA

May 2017
- Electrocatalysis for renewable energy via active-site engineering at the atomic scale

Seminar, University of South Carolina, Columbia, SC

Skills and Professional Activities

Teaching	Certified Software Carpentry instructor for workshops on introductory and advanced python for scientific computing. Served as lead or co-instructor in six eight-hour workshops, served as secondary instructor/helper in in five additional workshops. Developed workshop material for "Python as a Second Language" and "Introduction to Python with Gapminder Data" Twice served as instructor and course designer in the annual Materials Project Workshop. Served twice as TA to Prof. Eric Shaqfeh (Stanford ChemE) in "Applied Mathemetics for the Chemical and Biological Sciencies," an introductory graduate course for chemical engineers. Won outstanding TA award.
High-performance computing	Extensive experience in python software development for scientific applications. See my github profile. Experience using NERSC, Oak Ridge (OLCF), Argonne (ALCF), and SLAC supercomputing Resources. Extensive experience in automated workflow management. Contributor to pymatgen, FireWorks, atomate, and CatMAP open source projects
Data science	Extensive experience in MongoDB infrastructure for materials data management at the materials project. Experience using tensorflow, scikit-learn, pandas, jupyter and numerous other python libraries for data science.
DFT Simulations	Extensive experience using density functional theory software, including VASP, Quantum Espresso, GPAW, and Dacapo
Technical writing and reviewing	Experience in preparation of scientific manuscripts, research proposals, LaTeX, and data visualization Reviewed articles in ACS Catalysis (5), J. Phys. Chem. (1), Chem. Mater. (3), and Catalysis Today (1)

Hobbies and other interests

Music	Advanced proficiency in jazz vibraphone, completed coursework in jazz improvisation, jazz standards for gigs, and current member of *Music of the Masters* ensemble at California Jazz Conservatory's Community Jazz School. Collegiate proficiency in classical piano. Earned a performance certificate from two recitals given while at University of South Carolina in the studio of Prof. Joseph Rackers. Intermediate proficiency in steel drumming, 3 years experience in Palmetto Pans Steel Drum ensemble.
Quiz Bowl	Experienced moderator, player, and question writer for ACF and NAQT format team academic buzzer-based competitions, formerly for University of South Carolina and Stanford, currently serves as a volunteer.