Andrew J. Medford

Associate Professor
Georgia Institute of Technology
School of Chemical & Biomolecular Engineering
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Education

Stanford University

- ☐ *Doctor of Philosophy* - Chemical Engineering (Sept. 2015)
- ☐ *Master of Science* - Chemical Engineering (Sept. 2014)

North Carolina State University

- ☐ *Bachelor of Science* - Textile Engineering (May 2009)

Professional Positions

Georgia Institute of Technology

- ☐ *Associate Professor* - School of Chemical & Biomolecular Engineering (Aug. 2023 - Present)
- ☐ *Assistant Professor* - School of Chemical & Biomolecular Engineering (Jan. 2017 - Aug. 2023)

Georgia Institute of Technology

- ☐ *Postdoctoral Researcher* - School of Mechanical Engineering (Oct. 2015 - Jan. 2017)

Selected Awards and Honors

- ☐ AIChE Himmelblau Award for Innovations in Computer-Based Chemical Engineering Education (co-winner, 2024)
- ☐ Georgia Tech Excellence Award in Online Teaching (2024)
- ☐ ACS CATL Division Early Career Award (2023)
- ☐ Georgia Tech Center for Teaching and Learning (CTL) Teaching Honor Roll (2023)
- ☐ Georgia Tech Curriculum Innovation Award (co-winner, 2022)
- ☐ AIChE "35 under 35" Award (2020)
- ☐ Georgia Tech CTL/BP Junior Faculty Teaching Excellence Award (2020)
- ☐ NSF CAREER Award - CBET Catalysis (2020)
- ☐ Sigma Xi Scientific Research Honor Society (2020)
- ☐ AFRL Materials Science and Engineering Data Challenge Grand Prize Project (May 2016)
- ☐ Outstanding Teaching Assistant Award (June 2012)
- ☐ National Defense Science and Engineering Graduate Research Fellow (September 2012 - September 2015)
- ☐ National Science Foundation Graduate Research Fellowship (August 2010 - September 2012)
- ☐ National Science Foundation Nordic Research Opportunity (July 2012 - September 2012)
- ☐ Department of Energy Computational Science Graduate Research Fellowship (2012 - Could not Accept)
- ☐ J. William Fulbright Fellowship - Risø National Labs, Denmark (August 2009 - June 2010)

Memberships and Activities

- ☐ Organized "Open-Source Software in Chemistry" ACS "Convergent Research Community" (Fall 2022 & 2023 meetings)
- ☐ Member of ChBE Diversity, Equity, and Inclusion committee (2021 - 2022)
- ☐ Co-organizer for "Complexity in Catalysis" session at ACS meeting (2021)
- ☐ Initiated "Data Science in Catalysis" and "Catalysis for Nitrogen Chemistry" sessions at AIChE meeting (2018, 2019)
- ☐ Chair of departmental IT committee (2019 - 2022) and institute HPC (PACE) advisory committee (2020 - 2021)
- ☐ Led development of "Materials Informatics 101" workshop (Sept. 2019, Oct. 2021)
- ☐ Organized "Data Carpentry" and "Software Carpentry" workshops (June 2018, May 2019)
- ☐ Serve-Learn-Sustain Energy Systems for Sustainable Communities Fellow (Fall 2017)
- ☐ Speaker at local AIChE chapter meeting (2017)
- ☐ ASEE Chemical Engineering Education Summer School Participant (2017)
- ☐ ChBE Graduate Recruiting Weekend Committee (2017-2019)
- ☐ American Institute of Chemical Engineers Member (2013 - Present)
- ☐ American Chemical Society Member (2017 - Present)
- ☐ Southeastern Catalysis Society Member (2017 - Present), Interim Secretary (2021), Webmaster (2018), local planning co-chair (2018, 2021, 2023)

Teaching Experience

ChBE 4745/6745 - Data Analytics for Chemical Engineers
Georgia Institute of Technology - Spring 2020, Fall 2020, Fall 2021, Fall 2022, Fall 2023

COE 3803 - Data Analytics for Engineers
Georgia Institute of Technology - Fall 2018, Fall 2019

ChBE 2120 - Numerical Methods
Georgia Institute of Technology - Fall 2017, Spring 2019, Spring 2022, Spring 2023

ChBE 4803/8803 - Advanced Data Analysis for Chemical Engineers
Georgia Institute of Technology - Spring 2018

VIP - Big Data & Quantum Mechanics (vertically-integrated research course)
Georgia Institute of Technology - Spring 2017 - Present

Publications

- ☐ Total Publications: 96 (Peer Reviewed)
- ☐ H-Index: 48 (Google Scholar)
- ☐ Total Citations: 11,907 (Google Scholar)

Publications are organized by major topics in the group followed by additional publications. Within each sub-section papers with first or corresponding authorship at Georgia Tech are listed first in reverse chronological order, followed by collaborative works and work prior to Georgia Tech (separated by a horizontal rule for clarity).

Electron Scale Methods: Exchange-Correlation and Electronic Structure Theory

* "Optimization of random phase approximation calculations for improved energies of molecules, solids, and surfaces"
N. K. Yu, J. Voss, A. J. Medford
arXiv preprint (Under review) arXiv:2602.05138 (2026)

96. "Real-space Hubbard-corrected density functional theory"
S. Bhowmik, A. J. Medford, P. Suryanarayana
The Journal of Chemical Physics 163(23) (2025)

95. "SPARC-X-API: Versatile Python interface for real-space density functional theory calculations"
Tian Tian, Lucas R. Timmerman, Shashikant Kumar, B. M. Comer, Andrew J. Medford, Phanish Suryanarayana
Journal of Open Source Software 10(110), 7747 (2025)

94. "Assessing Exchange-Correlation Functionals for Heterogeneous Catalysis of Nitrogen Species"
H. Kim, N.-K. Yu, N. Tian, A. J. Medford *Journal of Physical Chemistry C* (2024)

93. "Self-consistent convolutional density functional approximations: Application to adsorption at metal surfaces"
S. J. Sahoo, Q. Xu, X. Lei, D. Staros, G. R. Iyer, B. Rubenstein, P. Suryanarayana, A. J. Medford *ChemPhysChem* (2024)

92. "Ab-initio investigation of finite size effects in rutile titania nanoparticles with semilocal and nonlocal density functionals"
S. J. Sahoo, X. Jing, P. Suryanarayana, A. J. Medford *J. Phys. Chem. C* 126, 4, pp. 2121–2130 (2022)

91. "ElectroLens: Understanding Atomistic Simulations through Spatially-Resolved Visualization of High-Dimensional Features"
X. Lei, F. Hohman, D. H. Polo Chau, and A. J. Medford, *IEEE Visualization Conference (VIS)* 2019

90. "Design and analysis of machine learning exchange-correlation functionals via rotationally invariant convolutional descriptors"
X. Lei, A. J. Medford, *Physical Review Materials* 3 (6) 2019

89. “Spectral scheme for atomic structure calculations in density functional theory”
Sayan Bhowmik, John E. Pask, Andrew J. Medford, Phanish Suryanarayana
Computer Physics Communications 308, 109448 (2025)

88. “SPARC v2. 0.0: Spin-orbit coupling, dispersion interactions, and advanced exchange–correlation functionals”
B. Zhang, X. Jing, Q. Xu, S. Kumar, A. Sharma, L. Erlandson, S. J. Sahoo, E. Chow, A. J. Medford, J. E. Pask *Software Impacts* 20, pp. 100649 (2024)

87. “Soft and transferable pseudopotentials from multi-objective optimization”
M. F. Shojaei, J. E. Pask, A. J. Medford, P. Suryanarayana *Computer Physics Communications* 283, 108594 (2023)

86. “SPARC: Simulation Package for Ab-initio Real-space Calculations”
Q. Xu, A. Sharma, B. M. Comer, H. Huang, E. Chow, A. J. Medford, J. E. Pask, P. Suryanarayana *SoftwareX* 15 pp. 100709 (2021)

Atomic Scale Methods: Machine Learned Force Fields and Artificial Intelligence

* “Prospects for Using Artificial Intelligence to Understand Intrinsic Kinetics of Heterogeneous Catalytic Reactions”
A. J. Medford, T. N. Whittaker, B. Kreitz, D. W. Flaherty, J. R. Kitchin
Current Opinion in Chemical Engineering Accepted. (2026)

85. “Comparing classical and machine learning force fields for modeling deformation of metal–organic frameworks relevant for direct air capture”
Logan M. Brabson, Andrew J. Medford, David S. Sholl
The Journal of Physical Chemistry C 129, 16811–16825 (2025)

84. “D–MOPH–25: diverse MOF–molecule pairs for Henry’s constants prediction”
Sihoon Choi, David S. Sholl, Andrew J. Medford
Machine Learning: Science and Technology 6(3), 035058 (2025)

83. “Overcoming the chemical complexity bottleneck in on-the-fly machine learned molecular dynamics simulations”
L. R. Timmerman, S. Kumar, P. Suryanarayana, A. J. Medford *Journal of Physical Chemistry C* (2024)

82. “AmpTorch: A Python package for scalable fingerprint-based neural network training on multi-element systems with integrated uncertainty quantification”
M. Shuaibi, Y. Hu, ... A.J. Medford, Z. Ulissi *Journal of Open Source Software* 8 (2023)

81. “Robust and scalable uncertainty estimation with conformal prediction for machine-learned interatomic potentials”
Y. Hu, J. Musielewicz, Z. Ulissi, A. J. Medford *Machine Learning: Science and Technology* 3, 045028 (2022)

80. “Gaussian Approximation of Dispersion Potentials for Efficient Featurization and Machine Learning Predictions of Metal-Organic Frameworks”
S. Choi, D. S. Sholl, A. J. Medford *J. Chem. Phys.* 156 pp. 214108 (2022)

79. “A Universal Framework for for Featurization of Atomistic Systems”
X. Lei, A. J. Medford *J. Phys. Chem. Letters* 13 pp. 7911-7919 (2021)

78. “Application of Density Functional Tight Binding and Machine Learning to Evaluate the Stability of Biomass Intermediates on the Rh (111) Surface”
C. Chang, A. J. Medford *J. Phys. Chem. C* 125 pp. 18210–18216 (2021)

77. “Classification of biomass reactions and predictions of reaction energies through machine learning”
C. Chang, A. J. Medford *J. Chem. Phys.* 153 (4) pp. 044126 (2020)

76. “Extracting Knowledge from Data through Catalysis Informatics”
A. J. Medford, M. R. Kunz, S. M. Ewing, T. Borders, R. Fushimi *ACS Catalysis* 8 pp. 7403-7429 (2018)

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75. “Rational design of selective catalysts for ethylene hydroformylation via microkinetic modeling and universal neural network potentials”
Kento Sakai, Ippei Furikado, Andrew J. Medford
Journal of Catalysis 450, 116253 (2025)

74. “The Open DAC 2023 dataset and challenges for sorbent discovery in direct air capture”
A. Sriram, S. Choi, X. Yu, L. M. Brabson, A. Das, Z. Ulissi, M. Uyttendaele, A. J. Medford, D. S. Sholl *ACS Central Science* 10 5 pp. 923-941 (2024)

73. “Kohn–Sham accuracy from orbital-free density functional theory via Δ-machine learning”
S. Kumar, X. Jing, J. E. Pask, A. J. Medford, P. Suryanarayana *The Journal of Chemical Physics* 159 24 (2023)

72. “Automated Generation of Microkinetics for Heterogeneously Catalyzed Reactions Considering Correlated Uncertainties”
B. Kreitz, P. Lott, F. Studt, A. J. Medford, O. Deutschmann, C. F. Goldsmith *Angewandte Chemie International Edition* 62 (39), e202306514 (2023)

71. “Phase Stability of Large-Size Nanoparticle Alloy Catalysts at *Ab Initio* Quality Using a Nearsighted Force-Training Approach”
C. Zeng, S. J. Sahoo, A. J. Medford, A. A. Peterson *The Journal of Physical Chemistry C* 127 (50), 24360-24372 (2023)

Reactor Scale Methods: Transient Kinetic Data Analysis

70. “Micro-kinetic modeling of temporal analysis of products data using kinetics-informed neural networks”
D. Nai, G. S. Gusmão, Z. A. Kilwein, F. Boukouvala, A. J. Medford *Digital Discovery* 3, 2327-2340 (2024)

69. “Model-based design of temporal analysis of products (TAP) reactors: A simulated case study in oxidative propane dehydrogenation”
A. C. Yonge, G. S. Gusmão, R. Fushimi, A. J. Medford *Industrial & Engineering Chemistry Research* 63, 11, 4756-4770 (2024)

68. “Maximum-likelihood Estimators in Physics-Informed Neural Networks for High-dimensional Inverse Problems”
G. S. Gusmão, A. J. Medford *Computers & Chemical Engineering* 181 (2024)

67. “Quantifying the impact of temporal analysis of products reactor initial state uncertainties on kinetic parameters” A. Yonge, G. S. Gusmão, R. Batchu, M. R. Kunz, Z. Fang, R. Fushimi, A. J. Medford
AIChE Journal 68 pp. e17776 (cover article) (2022)

66. “Kinetics-Informed Neural Networks”
G. S. Gusmao, A. P. Retnanto, S. C. da Cunha, A. J. Medford *Catalysis Today* 417 pp. 113701 (2022)

65. “TAPsolver: A Python package for the simulation and analysis of TAP reactor experiments”
A. Yonge, M. R. Kunz, R. Batchu, Z. Fang, T. Issac, R. Fushimi, A. J. Medford *Chemical Engineering Journal* 420 pp. 129377 (2021)

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64. “Internal calibration of transient kinetic data via machine learning”
M. R. Kunz, A. Yonge, X. He, R. Batchu, Z. Fang, Y. Wang, G. S. Yablonsky, A. J. Medford, R. Fushimi *Catalysis Today* 417, 113650 (2023)

63. “Training Stiff Dynamic Process Models via Neural Differential Equations”
W. Bradley, G. S. Gusmão, A. J. Medford, F. Boukouvala *Computer Aided Chemical Engineering* 49, 1741-1746 (2022)

62. “Internal Calibration of Transient Kinetic Data via Machine Learning”
M. R. Kunz, A. Yonge, X. He, R. Batchu, Z. Fang, Y. Wang, G. S. Yablonsky, A. J. Medford, R. R. Fushimi *Catalysis Today* (2022)

61. “Data Driven Reaction Mechanism Estimation via Transient Kinetics and Machine Learning”
M. R. Kunz, A. Yonge, Z. Fang, A. J. Medford, D. Constales, G. Yablonsky, R. Fushimi *Chem. Eng. J.* 420 pp. 129610 (2021)

Societal Considerations: Sustainable Ammonia Synthesis

60. "Formation of carbon-induced nitrogen-centered radicals on titanium dioxide under illumination"
P.-W. Huang, N. Tian, T. Rajh, Y.-H. Liu, G. Innocenti, C. Sievers, A.J. Medford, M. C. Hatzell *JACS Au* 3, 12, 3283–3289 (2023)

59. "Screening and discovery of metal compound active sites for strong and selective adsorption of N_2 in air"
N. Tian, B. M. Comer, A. J. Medford *ChemSusChem*, e202300948 (2023)

58. "Computational Study of Transition-Metal Substitutions in TiO_2(110) for Photoelectrocatalytic Ammonia Synthesis"
B. M. Comer, M. H. Lenk, A. P. Rajanala, E. L. Flynn, A. J. Medford *Catalysis Letters* (2020)

57. "Prospects and Challenges for Solar Fertilizers"
B. M. Comer, C. O. Dimkpa, Y.-H. Liu, C. A. Fernandez, P. Arora, M. Realff, U. Singh, M. C. Hatzell, A. J. Medford *Joule* 3 pp. 1578-1605 (2019)

56. "The Role of Adventitious Carbon in Photo-catalytic Nitrogen Fixation by Titania"
B. M. Comer, Y.-H. Liu, M. B. Dixit, K. B. Hatzell, Y. Ye, E. J. Crumlin, M. C. Hatzell, A. J. Medford *Journal of the American Chemical Society* 45 pp. 15157-15160 (2018)

55. "Analysis of photocatalytic nitrogen fixation on rutile TiO_2 (110)"
B.M. Comer, A. J. Medford *ACS Sustainable Chemistry & Engineering* 6 pp. 4648-4660 (2018)

54. "Photon-driven Nitrogen Fixation: Current Progress, Thermodynamic Considerations, and Future Outlook"
A. J. Medford, M. C. Hatzell *ACS Catalysis* 7 pp. 2624-2643 (2017)

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53. "Innovative approach to sustainable fertilizer production: Leveraging electrically assisted conversion of sewage sludge for nutrient recovery"
Gerardine G. Botte, Dayana Donneys-Victoria, Christian E. Alvarez-Pugliese, Jedidian Adjei, Selin Sahin, Nathan W. Wilson, Kayleigh Millerick, Amy Hardberger, Ariel L. Furst, Nicole Hu, Andrew J. Medford
ACS Omega 9(50), 49692–49706 (2024)

52. "Benchmarking photocatalysts for dinitrogen photoreduction reaction"
P. Huang, D. A. C. Haro, H. Song, A. J. Medford, M. C. Hatzell *Chem Catalysis* 4 (2024)

51. "Electrocatalysts for Inorganic and Organic Waste Nitrogen Conversion"
D. A. Chipoco Haro, L. Barrera, H. Iriawan, A. Herzog, N. Tian, A. J. Medford, Y. Shao-Horn, F. M. Alamgir, M. C. Hatzell *ACS Catalysis* 14, pp. 9752-9775 (2024)

50. "Impact of Local Microenvironments on the Selectivity of Electrocatalytic Nitrate Reduction in a BPM-MEA System"
P. W. Huang, H. Song, J. Yoo, D. A. Chipoco Haro, H. M. Lee, A. J. Medford, M. Hatzell *Advanced Energy Materials*, 2304202 (2024)

49. "6–Electrochemical & Photochemical ammonia synthesis/Electrochemical nitrate reduction"
D. R. MacFarlane, A. N. Simonov, A. J. Medford, M. Hatzell *2023 Roadmap on Ammonia as a Carbon-Free Fuel*

48. "Perspectives on the Competition between the Electrochemical Water and N_2 Oxidation on a TiO_2(110) Electrode"
E. Tayyebi, A. B. Hoskuldsson, A. Wark, N. Atrak, B. M. Comer, A. J. Medford, E. Skulason *J. Phys. Chem. Letters* 13 pp. 6123-6129 (2022)

47. "Methods for nitrogen activation by reduction and oxidation"
H. Iriawan, S. Z. Andersen, X. Zhang, B. M. Comer, J. Barrio, P. Chen, A. J. Medford, I. E. L. Stephens, I. Chorkendorff, Y. Shao-Horn *Nature Reviews Methods Primer* 1, pp. 1-26 (2021)

46. "Mechanocatalytic Ammonia Synthesis over TiN in Transient Microenvironments"
A. W. Tricker, K. L. Hebisch, M. Buchmann, Y.-H. Liu, M. Rose, E. Stavitski, A. J. Medford, M. C. Hatzell, and C. Sievers *ACS Energy Letters* pp. 3362–3367 (2020)

45. "Assessing the reliability of calculated catalytic ammonia synthesis rates"
A. J. Medford, J. Wellendorff, A. Vojvodic, F. Studt, F. Abild-Pedersen, K. W. Jacobsen, T. Bligaard, J. K. Nørskov *Science* 345 (2014) pp. 197-200

44. "Exploring the limits: A low-pressure, low-temperature Haber-Bosch process"
A. Vojvodic, A. J. Medford, F. Studt, F. Abild-Pedersen, T. S. Khan, T. Bligaard, J. K. Nørskov *Chemical Physics Letters* 598 (2014) pp. 108-112

Additional Publications

43. "Evaluating the role of metastable surfaces in mechanochemical reduction of molybdenum oxide"
N.-K. Yu, L. Rasteiro, V.S. Nguyen, K. Golabek, C. Sievers, A.J. Medford *JACS Au* Accepted (2024)

42. "Unifying thermochemistry concepts in computational heterogeneous catalysis"
B. Kreitz, G. S. Gusmão, D. Nai, S. J. Sahoo, A. A. Peterson, D. H. Bross, C. F. Goldsmith, A. J. Medford *Chemical Society Reviews* Accepted (2024)

41. "Online Graduate Certificate in Data Science for the Chemical Industry"
A.J. Medford, F. Boukouvala, *et al. Chemical Engineering Education* 56 (2022)

40. "A Career in Catalysis: Jens Kehlet Nørskov"
A. J. Medford, P. G. Moses, K. W. Jacobsen, A. A. Peterson *ACS Catal.* 12 pp. 9679-9689 (2022)

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39. "Ab initio study of strain-driven vacancy clustering in aluminum"
Sayan Bhowmik, Andrew J. Medford, Phanish Suryanarayana, Abhiraj Sharma
Physical Review B 112, 174110 (2025)

38. "Boron-tuned tetrahedral Co(II) sites in zeolite Beta enhance propane dehydrogenation"
Younhwa Kim, Huston Locht, Andrew J. Medford, Christopher W. Jones
Applied Catalysis B: Environmental 382, 126077 (2025)

37. "Role of Catalyst Domain Size in the Hydrogenation of CO_2 to Aromatics over ZnZrOx/ZSM-5 Catalysts"
I. Nezam, W. Zhou, D. R. Shah, M.P. Bukhovko, M. R. Ball, G. S. Gusmão, A. J. Medford, C. W. Jones *The Journal of Physical Chemistry C* 127 (13), 6356-6370 (2023)

36. "Surface Interactions of Erythrose on Assorted Metal Oxides: A Solid-State NMR Study"
S. Najmi, C. L. Liotta, A. J. Medford, C. Sievers *The Journal of Physical Chemistry C* 127 (3), 1430-1440 (2023)

35. "Efficient Models for Predicting Temperature-Dependent Henry's Constants and Adsorption Selectivities for Diverse Collections of Molecules in Metal–Organic Frameworks"
X. Yu, S. Choi, D. Tang, A. J. Medford, D. S. Sholl *J. Phys. Chem. C* 125, pp. 18046–18057 (2021)

34. "Heterogeneity in susceptibility dictates the order of epidemiological models"
C. Rose, A. J. Medford, C. F. Goldsmith, T. Vegge, J. S. Weitz, A. A. Peterson *J. Theoretical Biology* 528, pp. 110839 (2021)

33. "Continuous Liquid-Phase Upgrading of Dihydroxyacetone to Lactic Acid over Metal Phosphate Catalysts"
G. Innocenti, E. Papadopoulos, G. Fornasari, F. Cavani, A. J. Medford, and C. Sievers *ACS Catal.* 10 (20) pp. 11936–11950 (2020)

32. "Pretreatment Effects on the Surface Chemistry of Small Oxygenates on Molybdenum Trioxide"
S. Najmi, M. Rasmussen, G. Innocenti, C. Chang, E. Stavitski, S. R. Bare, A. J. Medford, J. W. Medlin, and C. Sievers *ACS Catal.* 10 (15) pp. 8187–8200 (2020)

31. "Database of Computation-Ready 2D Zeolitic Slabs"
O. Knio, A. J. Medford, S. Nair, D. S. Sholl *Chemistry of Materials* 31 pp. 353-364 (2019)

30. "Thermodynamic Limitations of the Catalyst Design Space for Methanol Production from Methane"
J. N. Joscz, A. J. Medford, C. Sievers *ChemCatChem* 11 pp. 593-600 (2019)

29. "Selectivity of Synthesis Gas Conversion to C_{2+} Oxygenates on fcc(111) Transition-Metal Surfaces"
J. Schumann, A. J. Medford, J. S. Yoo, Z.-J. Zhao, P. Bothra, A. Cao, F. Studt, F. Abild-Pedersen, and J. K. Nørskov *ACS Catalysis* 8 pp. 3447-3453 (2018)

28. "Extracting Knowledge from Molecular Mechanics Simulations of Grain Boundaries Using Machine Learning"
J. A. Gomberg, A. J. Medford, S. K. Kalidindi *Acta Materialia* 133 pp. 100-108 (2017)

27. "Vision for Data and Informatics in the Future Materials Innovation Ecosystem"
S. R. Kalidindi, A. J. Medford, D. L. McDowell *JOM* (2016) 68 pp. 2126-2137

26. "Scaling-Relation-Based Analysis of Bifunctional Catalysis: The Case for Homogeneous Bimetallic Alloys"
M. Andersen, A. J. Medford, J. K. Nørskov, K. Reuter *ACS Catalysis* 7 pp. 3960-3967 (2017)

25. "To address surface reaction network complexity using scaling relations machine learning and DFT calculations"
Z. W. Ulissi, A. J. Medford, T. Bligaard, and J. K. Norskov *Nature Communications* (2017)

24. "Framework for Scalable Adsorbate-Adsorbate Interaction Models"
M. J. Hoffmann, A. J. Medford, T. Bligaard *Journal of Physical Chemistry C* (2016) 120 pp. 13087-13094

23. "Analyzing the Case for Bifunctional Catalysis"
M. Andersen, A. J. Medford, J. K. Nørskov, K. Reuter *Angewandte Chemie* (2016) 55 pp. 5210-5214

22. "On the Intrinsic Selectivity and Structure Sensitivity of Rhodium Catalysts for C_{2+} Oxygenate Production"
N. Yang, A. J. Medford, X. Liu, F. Studt, T. Bligaard, S. Bent, J. K. Nørskov *Journal of the American Chemical Society* (2016) 138 pp. 3705-3714

21. "From the Sabatier principle to a predictive theory of transition-metal heterogeneous catalysis"
A. J. Medford, A. Vojvodic, J. S. Hummelshøj, J. Voss, F. Abild-Pedersen, F. Studt, T. Bligaard, A. Nilsson, J. K. Nørskov *Journal of Catalysis* (2015) 328 pp. 36-42

20. "CatMAP: A software package for descriptor-based micro-kinetic mapping of catalytic trends"
A. J. Medford, C. Shi, M. J. Hoffmann, A. C. Lausche, S. Fitzgibbon, T. Bligaard, J. K. Nørskov *Catalysis Letters* (2105) 145 pp. 794-807

19. "Degree of rate control approach to computational catalyst screening"
C. A. Wolcott, A. J. Medford, F. Studt, C. T. Campbell *Journal of Catalysis* (2015) 330 pp. 197-207

18. "Departures from the adsorption energy scaling relations for metal carbide catalysts"
R. Michalsky, Y. Zhang, A. J. Medford, A. A. Peterson *Journal of Physical Chemistry C* 118 (2014) pp. 13026-13034

17. "Activity and selectivity trends in synthesis gas conversion to higher alcohols"
A. J. Medford, A. C. Lausche, F. Abild-Pedersen, B. Temel, N. C. Schjødt, J. K. Nørskov, F. Studt *Topics in Catalysis* 57 (2014) pp. 135-142

16. "Thermochemistry and micro-kinetic analysis of methanol synthesis on ZnO(0001)"
A. J. Medford, J. Sehested, J. Rossmeisl, I. Chorkendorff, F. Studt, J. K. Nørskov, P. G. Moses *Journal of Catalysis* 309 (2014) pp. 397-407

15. "On the effect of coverage-dependent adsorbate-adsorbate interactions for CO methanation on transition metal surfaces"
A. C. Lausche, A. J. Medford, T. S. Khan, Y. Xu, T. Bligaard, F. Abild-Pedersen, J. K. Nørskov, F. Studt *Journal of Catalysis* 307 (2013) pp. 275-282

14. "Finite-size effects in O and CO adsorption for the late transition metals"
A. A. Peterson, L. C. Grabow, T. P. Brennan, B. Shong, C. Ooi , D. M. Wu, C. W. Li, A. Kushwaha, A. J. Medford, F. Mbuga, L. Li, J. K. Nørskov *Topics in Catalysis* 55 (2012) pp. 1276-1282

13. "Elementary steps of syngas reactions on $Mo_2C(001)$: Adsorption thermochemistry and bond dissociation"
A. J. Medford, A. Vojvodic, F. Studt, F. Abild-Pedersen, J. K. Nørskov *Journal of Catalysis* 290 (2012) pp. 108-117

12. "Electrocatalytic interaction of nano-engineered palladium on carbon nanofibers with hydrogen peroxide and β-NADH"
Z. Lin, L. Ji, A. J. Medford, Q. Shi, W. E. Krause, X. Zhang *Journal of Solid State Electrochemistry* 15 (2011) pp. 1287-1294

11. “An inter-laboratory stability study of roll-to-roll coated flexible polymer solar modules”
S. A. Gevorgyan, A. J. Medford, E. Bundgaard, F. C. Krebs *et. al. Solar Energy Materials and Solar Cells* 95 (2011) pp. 1398-1416

10. “Ultra-fast and parsimonious materials screening for polymer solar cells using differentially pumped slot-die coating”
J. Alstrup, M. Jørgensen, A. J. Medford, F. C. Krebs *ACS Applied Materials and Interfaces* 2 (2011) pp. 2819-2827

9. “The effect of post-processing treatments on inflection points in current-voltage curves of roll-to-roll processed polymer photovoltaics”
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