

Matthew M. Montemore

POSTDOCTORAL SCHOLAR, HARVARD UNIVERSITY

John A. Paulson School of Engineering and Applied Sciences · Department of Chemistry and Chemical Biology

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Research Interests and Accomplishments

RESEARCH INTERESTS

Applications: Catalysis, electrochemistry, energy conversion, and energy transport in interfaces and nanostructures.
Methods: Performing quantum simulations; developing and applying semiempirical models; machine learning and data science.

RESEARCH ACCOMPLISHMENTS

Showed that reactions on metal surfaces can induce electronic excitations, which can affect surface chemistry.
Performed kinetic, thermodynamic, and multiscale modelling studies to explain catalytic performance and materials synthesis for alloys.
Developed a general model for predicting adsorption on transition metals, which is useful for efficient catalyst design.
Currently using high-throughput computation and machine learning to understand and design novel alloy catalysts.

Education and Research Experience

Harvard University

POSTDOCTORAL SCHOLAR, Department of Chemistry, School of Engineering and Applied Sciences

November 2014 to present

Advisor: Efthimios Kaxiras

University of Colorado Boulder

PH.D., Mechanical Engineering

August 2014

Dissertation: Designing Transition Metal Surfaces for their Adsorption Properties and Chemical Reactivity

Advisors: J. Will Medlin (Chemical Engineering), John W. Daily (Mechanical Engineering)

M.S., Mechanical Engineering

May 2011

Grinnell College

B.A., Physics, w/honors

May 2009

University of Chicago

RESEARCH EXPERIENCE FOR UNDERGRADUATES, Materials Research Science and Engineering Center

Summer 2008

Advisor: Thomas A. Witten

Publications

Published (18 total, 11 first author)

- 1 **M. M. MONTEMORE**, M. A. VAN SPRONSEN, R. J. MADIX, C. M. FRIEND. O₂ Activation by Metal Surfaces: Implications for Bonding and Reactivity on Heterogeneous Catalysts. *Accepted to Chemical Reviews*.
- 2 **M. M. MONTEMORE**, A. MONTESSORI, S. SUCCI, C. BARROO, G. FALCUCCI, D. C. BELL, E. KAXIRAS. Effect of nanoscale flows on the surface structure of nanoporous catalysts. *J. Chem. Phys.* 146 (2017) 214703 [[Link](#)]
- 3 C. BARROO, **M. M. MONTEMORE**, N. JANVELYAN, B. ZUGIC, A. AKEY, A. P. MAGYAR, J. YE, E. KAXIRAS, J. BIENER, D. C. BELL. Chemistry-driven Kirkendall effect and the formation of 3D nanoporosity. *J. Phys. Chem. C* 121 (2017) 5115 [[Link](#)]
- 4 **M. M. MONTEMORE**, E. D. CUBUK, J. E. KLOBAS, M. SCHMID, R. J. MADIX, C. M. FRIEND, E. KAXIRAS. Controlling O coverage and stability by alloying Au and Ag. *Phys. Chem. Chem. Phys.* 18 (2016) 26844 [[Link](#)]
- 5 **M. M. MONTEMORE**, O. ANDREUSSI, AND J. W. MEDLIN. Hydrocarbon Adsorption in an Aqueous Environment: A Computational Study of Alkyls on Cu(111). *J. Chem. Phys.* 145 (2016) 074702 [[Link](#)]
- 6 **M. M. MONTEMORE**, R. J. MADIX, E. KAXIRAS. How does nanoporous gold dissociate molecular oxygen? *J. Phys. Chem. C* 120 (2016) 16636 [[Link](#)]
- 7 M. L. PERSONICK, **M. M. MONTEMORE**, E. KAXIRAS, R. J. MADIX, J. BIENER, C. M. FRIEND. Catalyst design for enhanced sustainability through fundamental surface chemistry. *Philos. Trans. R. Soc. A* 374 (2016) 20150077 [[Link](#)] (Chosen for cover)
- 8 F. HIEBEL, **M. M. MONTEMORE**, E. KAXIRAS, C. M. FRIEND. Direct visualization of quasi-ordered oxygen chain structures on Au(110)-(1×2) *Surf. Sci.* 650 (2015) 5 [[Link](#)]

- 9 J. W. MEDLIN AND **M. M. MONTEMORE**. Scaling the rough heights. *Nat. Chem.* 7 (2015) 378 [\[Link\]](#)
- 10 T. D. GOULD, **M. M. MONTEMORE**, A. LUBERS, L. D. ELLIS, J. FALCONER, J. W. MEDLIN. Enhanced Dry Reforming of Methane on Ni and Ni-Pt Catalysts Synthesized by Atomic Layer Deposition. *Appl. Catal. A* 492 (2015) 107 [\[Link\]](#)
- 11 **M. M. MONTEMORE** AND J. W. MEDLIN. A Unified Picture of Adsorption on Transition Metals Through Different Atoms. *J. Am. Chem. Soc.* 136 (2014) 9272 [\[Link\]](#) (**Communication, chosen for JACS Spotlight** [\[Link\]](#))
- 12 **M. M. MONTEMORE** AND J. W. MEDLIN. Scaling Relations Between Adsorption Energies for Computational Screening and Design of Catalysts. *Catal. Sci. & Technol.* 4 (2014) 3748 [\[Link\]](#)
- 13 **M. M. MONTEMORE** AND J. W. MEDLIN. Predicting and Comparing C–M and O–M Bond Strengths for Adsorption on Transition Metal Surfaces. *J. Phys. Chem. C* 118 (2014) 2666 [\[Link\]](#)
- 14 A. M. ROBINSON, **M. M. MONTEMORE**, S. A. TENNEY, P. SUTTER, J. W. MEDLIN. Interactions of Hydrogen, CO, Oxygen, and Water with Molybdenum-Modified Pt(111). *J. Phys. Chem. C* 117 (2013) 26716 [\[Link\]](#)
- 15 **M. M. MONTEMORE** AND J. W. MEDLIN. Site-Specific Scaling Relations for Hydrocarbons on Hexagonal Transition Metal Surfaces. *J. Phys. Chem. C* 117 (2013) 20078 [\[Link\]](#)
- 16 M. B. GRIFFIN, A. A. RODRIQUEZ, **M. M. MONTEMORE**, J. R. MONNIER, C. T. WILLIAMS, J. W. MEDLIN. The selective oxidation of ethylene glycol and 1,2-propanediol on Au, Pd, and Au–Pd bimetallic catalysts. *J. Catal.* 307 (2013) 111 [\[Link\]](#)
- 17 **M. M. MONTEMORE** AND J. W. MEDLIN. A Simple, Accurate Model for Alkyl Adsorption on Late Transition Metals. *J. Phys. Chem. C* 117 (2013) 2835 [\[Link\]](#)
- 18 **M. M. MONTEMORE** AND J. W. MEDLIN. A Density Functional Study of C₁–C₄ Alkyl Adsorption on Cu(111). *J. Chem. Phys.* 136 (2012) 204710 [\[Link\]](#)

Submitted

- 19 **M. M. MONTEMORE**, R. HOYT, G. KOLESOV, E. KAXIRAS. Reaction-Induced Excitations and their Effect on Surface Chemistry. *Submitted to Nature Chem.*

In Preparation

- 20 **M. M. MONTEMORE**, B. LY, E. D. CUBUK, E. KAXIRAS. Machine learning for structural predictions of AgAu surfaces in oxidizing atmospheres. *In Preparation.*
- 21 **M. M. MONTEMORE**, M. VAN SPRONSEN, N. JANVELYAN, M. PERSONICK, R. J. MADIX, C. M. FRIEND, E. KAXIRAS. Surface reconstruction prevents O₂ dissociation on gold. *In Preparation.*
- 22 **M. M. MONTEMORE***, R. HOYT*, I. FAMPIOU, T. SMIDT, K. KOHLHOFF, P. RILEY, G. TRITSARIS, E. KAXIRAS [* DENOTES EQUAL CONTRIBUTIONS]. Selective Hydrogenation Catalyst Discovery through Data Mining and Machine Learning. *In Preparation.*

Fellowships and Proposals

Grant-Writing Experience and Training

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|---|------|
| ASSISTED WITH IMASC EFRC RENEWAL PROPOSAL | 2017 |
| COMPLETED “SUCCESSFUL GRANT WRITING STRATEGIES”, online course through Harvard University | 2016 |

Computational Proposals

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| AWARDED 17.5 MILLION PROCESSOR HOURS THROUGH ALCC, Oak Ridge Leadership Computing Facility | 2016 |
| WROTE 15-PAGE PROPOSAL | |
| ALCF DIRECTOR’S DISCRETIONARY ALLOCATION. LEAD PROPOSAL PREPARATION. | 2014 |
| OLCF DIRECTOR’S DISCRETIONARY ALLOCATION. LEAD PROPOSAL PREPARATION. | 2014 |
| NERSC SUPERCOMPUTING NETWORK, DOE | 2014–2017 |
| JANUS SUPERCOMPUTER, CU Boulder | 2011–2013 |
| XSEDE SUPERCOMPUTING NETWORK, NSF | 2011–2012 |
| CHINOOK SUPERCOMPUTER, Pacific Northwest National Lab | 2011–2012 |
| CARBON SUPERCOMPUTER, Argonne National Lab | 2011–2013 |
| TERAGRID SUPERCOMPUTING NETWORK, NSF | 2011 |

Fellowships

CARL STORM UNDERREPRESENTED MINORITY FELLOWSHIP, Gordon Research Conference on Catalysis	2014
FELLOWSHIP GRANT, Colorado Center for Biorefining and Bioproducts	2013
WROTE PROPOSAL	
BASF FELLOWSHIP, North American Catalysis Society	2012
AGEP FELLOWSHIP, NSF	2009–2010
DIVERSITY FELLOWSHIP, CU Boulder	2009

Presentations

Invited Talks and Seminars

NONADIABATIC EFFECTS AND ELECTRONIC EXCITATIONS DURING DISSOCIATION ON CATALYTIC SURFACES	2016
Invited Talk at Fall ACS National Meeting, Philadelphia	
NONADIABATIC EFFECTS IN DISSOCIATION ON TRANSITION METAL SURFACES	2016
Invited Talk at Spring ACS National Meeting, San Diego	
HOW DOES NANOPOROUS AU DISSOCIATE O ₂ ?	2016
Invited Talk at Spring ACS National Meeting, San Diego	
COMPUTATIONAL UNDERSTANDING AND DESIGN OF TRANSITION METAL CATALYSTS	2015
Seminar at Oak Ridge National Laboratory	

Selected Conference Talks (out of 13 total)

<i>In Situ</i> SURFACE STRUCTURE OF BIMETALLIC NANOPOROUS CATALYSTS—THE EFFECT OF NANOSCALE FLOW	2017
To be given at Fall MRS Meeting, Boston	
ELECTRONIC EXCITATIONS IN THERMAL HETEROGENEOUS CATALYSIS	2017
To be given at AIChE National Meeting, Minneapolis	
DFT STUDIES OF THE STRUCTURE AND REACTIVITY OF AGAU ALLOYS	2015
Fall ACS National Meeting, Boston	
PREDICTING ADSORPTION ENERGIES FOR USE IN CATALYST DESIGN	2014
AIChE National Meeting, Atlanta	

Selected Conference Poster Presentations (out of 8 total)

ELECTRONIC EXCITATIONS IN THERMAL HETEROGENEOUS CATALYSIS	2017
American Conference on Theoretical Chemistry	
FAST PREDICTIONS OF ADSORPTION ENERGIES FOR EFFICIENT CATALYST DESIGN	2014
Gordon Research Conference on Catalysis, New Hampshire	
THEORY OF HYDROCARBON ADSORPTION ON TRANSITION METAL SURFACES	2013
North American Catalysis Society North American Meeting, Louisville	
DFT STUDY OF ALKYL ADSORPTION AND SOLVATION ON TRANSITION METALS	2012
International Congress on Catalysis, Munich, Germany	

Grant Review Presentations, PI Meeting Presentations, and Seminars

HOW DOES NANOPOROUS AU DISSOCIATE O ₂ ?	2016
Oral and poster presentations at EFRC mid-term review, Washington DC	
HIGH-THROUGHPUT COMPUTATION AND MACHINE LEARNING FOR UNDERSTANDING AND DESIGNING CATALYSTS	2016
Poster presentation at Materials Genome Initiative PI Meeting, Washington DC	
HOW DOES NANOPOROUS AU DISSOCIATE O ₂ ?	2015
Poster presentation at EFRC PI Meeting, Washington DC	

Teaching and Mentoring

Teaching

HARVARD UNIVERSITY, TEACHING ASSISTANT
Chem 265 Surface and Interfacial Phenomena
AC 275 Computational Materials Design

Spring 2017

Spring 2015

UNIVERSITY OF COLORADO BOULDER, PART-TIME LECTURER
Physics, Upward Bound program

Summer 2013

Designed curriculum, lectures, homework, and format for class of Native American high school students

GRINNELL COLLEGE, LAB ASSISTANT AND TUTOR
Lab Assistant for General Physics I

2008

Tutor for General Physics I, General Physics II and The Universe and its Structure

2007–2009

Mentoring

4 UNDERGRADUATE RESEARCHERS, in Medlin and Kaxiras groups

2011, 2014, 2016, 2017

4 GRADUATE STUDENTS AND 3 POSTDOCS, in Medlin and Kaxiras groups

2014–2017

MENTOR FOR SUMMER MULTICULTURAL ACCESS TO RESEARCH TRAINING (SMART) PROGRAM (5 COHORTS)

2010–2014

MENTOR FOR COLORADO ADVANTAGE (3 COHORTS), a grad school preview program for underrepresented undergrads

2011–2013

TUTORED AND MENTORED AT-RISK LATINO STUDENTS (3 COHORTS), Adelante program at Boulder High School

2010–2013

Awards, Service, and Professional Development

Awards

NOMINATED FOR BEST PAPER, AIChE conference, Atlanta

Fall 2014

HELPED MEDLIN GROUP WIN DEAN'S PERFORMANCE AWARD FOR RESEARCH, from CU College of Engineering

2014

AWARDED PRIZE FOR THIRD PLACE, Western States Catalysis Club

April 2013

AWARDED PRIZES, CU Mechanical Engineering Graduate Engineering Annual Research & Recruiting Symposium

2012 & 2014

Service

CHAIR, Computational Catalysis session, AIChE National Meeting

2017

REVIEWER, ACS, RSC, Elsevier, NPG, World Scientific, AIP

2015–present

CO-ORGANIZER, IMASC Student/Postdoc Symposium

2016

IMASC REPRESENTATIVE, EFRC Early Career Network

2016–2017

ORGANIZING COMMITTEE, Graduate Engineering Annual Research & Recruiting Symposium

2011–2012

Workshops and Professional Development

CHOSEN FOR ACS POSTDOC TO FACULTY WORKSHOP

Fall 2016

ATTENDED INSTITUTE ON TEACHING AND MENTORING, a conference sponsored by The Compact for Faculty Diversity

2010