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Curriculum Vitae

JOHN MARK P. MARTIREZ

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Department of Chemical and Biomolecular Engineering
University of California, Los Angeles
Los Angeles, California, USA 90095
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Education

2015 — **Ph.D. in Chemistry (Physical)**
Advisor: **Prof. Andrew M. Rappe**
University of Pennsylvania
Philadelphia, Pennsylvania, United States

Research Activities and Interests

Application of quantum mechanical methods (density functional theory and multiconfigurational correlated wavefunction or post Hartree-Fock theories, e.g., CASSCF, CASPT2, and NEVPT2) to understand and design functional (nano)materials, focusing on materials for sustainable energy conversion technologies and green chemical processing

Recent Award

2020 American Chemical Society, Physical Chemistry Division Young Investigator Award

Professional Appointments

Assistant Project Scientist – Engineering, step 2 (September 2019 – present)
Supervisor: **Prof. Emily A. Carter** (Executive Vice Chancellor and Provost)
University of California, Los Angeles
Los Angeles, California, United States
Responsibilities:

- conduct research in the field of atomic-scale *ab initio* computational catalysis
- publish research in internationally recognized scientific journals
- help supervise graduate students and postdoctoral research associates in conducting their research
- help manage internal and external (provided by the US Department of Defense) computational resources
- oversee acquisition and compilation of software used by the research group
- participate in writing federal grant applications
- participate in writing federal grant reports and research updates
- present research at international and national scientific conferences and meetings

Associate Research Scholar (May 2018 – August 2019)
Supervisor: **Prof. Emily A. Carter** (Dean of the School of Engineering and Applied Science)
Princeton University
Princeton, New Jersey, United States
Responsibilities:

- conduct research in the field of atomic-scale *ab initio* computational catalysis
- publish research in internationally recognized scientific journals
- help supervise graduate students and postdoctoral research associates in conducting their research
- help manage internal and external (provided by the US Department of Defense) computational resources
- oversee acquisition and compilation of software used by the research group
- participate in writing federal grant applications
- participate in writing federal grant reports and research updates
- present research at international and national scientific conferences and meetings

Postdoctoral Research Associate (March 2015 – April 2018)
Supervisor: **Prof. Emily A. Carter (**Dean of the School of Engineering and Applied Science)
Princeton University
Princeton, New Jersey, United States
Responsibilities:

- conduct research in the field of atomic-scale *ab initio* computational catalysis
- publish research in internationally recognized scientific journals
- help supervise undergraduate and graduate students in conducting their research
- participate in writing federal grant applications
- participate in writing federal grant reports and research updates
- present research at international and national scientific conferences and meetings

University Instructor, rank 4 (June 2006 – May 2008)
Institute of Chemistry, College of Science
University of the Philippines,
Diliman, Quezon city, Metro Manila, Philippines
Responsibilities:

- teach laboratory courses in general, analytical, organic, and physical chemistry
- grade laboratory reports
- prepare and grade practical and written laboratory exams
- help prepare laboratory manuals and class syllabi

Patents

4. L. Li, J. M. P. Martirez and E. A. Carter, Mo-doped graphene-like GaN monolayer as electrocatalyst for artificial ammonia synthesis via nitrogen reduction reaction. ***Provisional US patent application no*. 63/033,325** (filed on June 2, 2020)
3. J. M. P. Martirez and E. A. Carter, Fe-Cu and Fe-Ag as primary-secondary co-dopants into NiOOH for enhanced electrochemical molecular oxygen evolution catalysis. ***Provisional US patent application no*. 62/948,392** (filed on December 16, 2019)
2. J. M. P. Martirez and E. A. Carter, Plasmonic Haber-Bosch catalysts based on surface-doped Au nanoparticles. ***Provisional US patent application no*. 62/638,728** (filed on March 5, 2018)
1. J. M. P. Martirez, S. Kim, and A. M. Rappe, Synergistic Oxygen Evolving Activity of Non-Stoichiometric Surfaces. ***United States Letters Patent No*.: 9,469,908**. Issued October 18, 2016

Publications

29. L. Li, J. M. P. Martirez, and E. A. Carter, Prediction of Highly Selective Electrocatalytic Nitrogen Reduction at Low Overpotential on a Mo-doped g-GaN Monolayer. (2020) ***under peer review***
28. Q. Zhao, X. Zhang, J. M. P. Martirez, and E. A. Carter, Benchmarking an embedded adaptive sampling configuration interaction method for surface reactions: H_2 desorption from and CH_4 dissociation on Cu(111). (2020) ***under peer review***
27. *Review Article*: J. M. P. Martirez, J. L. Bao, and E. A. Carter, First Principles Insights into Plasmon-Induced Catalysis. **Annual Review of Physical Chemistry**, *accepted* (2020)
26. *Review Article*: A. G. Rajan, J. M. P. Martirez, and E. A. Carter, Why do we use the materials and operating conditions we use for heterogeneous (photo)electrochemical water splitting? **ACS Catalysis**, *in press* (2020) DOI: 10.1021/acscatal.0c01862
25. J. M. P. Martirez, and E. A. Carter, Secondary transition-metal dopants for enhanced electrochemical O_2 formation and desorption on Fe-doped β-NiOOH. **ACS Energy Letters**, **5**, 962-967 (2020) DOI: 10.1021/acsenergylett.9b02761
24. J. M. P. Martirez, and E. A. Carter, Noninnocent influence of host β-NiOOH redox activity on transition metal dopants' efficacy as active sites in electrocatalytic water oxidation. **ACS Catalysis**, **10**, 2720-2734 (2020) DOI: 10.1021/acscatal.9b05092
23. A. G. Rajan, J. M. P. Martirez, and E. A. Carter, Facet-Independent Oxygen Evolution Activity of Pure β-NiOOH: Different Chemistries Leading to Similar Overpotentials. **Journal of the American Chemical Society**, **142**, 3600-3612 (2020) DOI: 10.1021/jacs.9b13708
22. L. Zhou, J. M. P. Martirez, J. Finzel, C. Zhang, D. F. Swearer, S. Tian, H. Robatjazi, M. Lou, L. Dong, L. Henderson, P. Christopher, E. A. Carter, P. Nordlander, N. J. Halas, Light-driven methane dry reforming with single atomic site antenna-reactor plasmonic photocatalysts. **Nature Energy**, **5**, 61-70 (2020) DOI: 10.1038/s41560-019-0517-9

    - Featured in the ***Daily Bruin***: "UCLA researchers help develop improved process for synthesis gas production" by Zhichun Li, January 22, 2020
    - ***Chemical & Engineering News:*** "Light-activated catalyst makes syngas greener" by Leigh Krietsch Boerner, January 17, 2020.
    - ***Rice News***: "Rice's low-temp photocatalyst could slash the carbon footprint for syngas" by Jade Boyd, January 10, 2020.
    - ***Nature - Research Highlights***: "More light than heat helps turn greenhouse gases into valuable product" January 9, 2020.
    - UCLA newsroom: "A greener, simpler way to create syngas" by Mathew Chin, January 6, 2020.

21. D. F. Swearer, H. Robatjazi, J. M. P. Martirez, M. Zhang, L. Zhou, E. A. Carter, P. Nordlander, and N. J. Halas, Plasmonic Photocatalysis of Nitrous Oxide into N_2 and O_2 using Aluminum-Iridium Antenna-Reactor Nanoparticles. **ACS Nano, 13**, 8076-8086 (2019) DOI: 10.1021/acsnano.9b02924
20. J. M. P. Martirez, and E. A. Carter, Unraveling Oxygen Evolution on Iron-Doped β-Nickel Oxyhydroxide: the Key Role of Highly Active Molecular-like Sites. **Journal of the American Chemical Society**, **141**, 693-705 (2019) DOI: 10.1021/jacs.8b12386
19. Z. Chen,* J. M. P. Martirez,* P. Zahl, E. A. Carter, and B. E. Koel, Self-Assembling of Formic Acid on the Partially Oxidized *p*(2×1) Cu(110) Surface Reconstruction at Low Coverages. **The Journal of Chemical Physics, 150***,* 041720 (2019) DOI: 10.1063/1.5046697

18. A. J. Tkalych, J. M. P. Martirez, and E. A. Carter, Thermodynamic evaluation of trace-amount transition-metal ion doping in NiOOH films. **Journal of the Electrochemical Society, 165**, F907-F913 (2018) DOI: 10.1149/2.0101811jes
17. J. M. P. Martirez, and E. A. Carter, Effects of the Aqueous Environment on the Stability and Chemistry of β-NiOOH Surfaces. **Chemistry of Materials**, **30**, 5205-5219 (2018) DOI: 10.1021/acs.chemmater.8b01866
16. A. J. Tkalych, J. M. P. Martirez, and E. A. Carter, Effect of transition-metal-ion dopants on the oxygen evolution reaction on NiOOH(0001). **Physical Chemistry and Chemical Physics**, **20,** 19525-19531 (2018) DOI: 10.1039/C8CP02849D
15. L. D. Chen, M. Bajdich, J. M. P. Martirez, C. M. Krauter, J. A. Gauthier, E. A. Carter, A. C. Luntz, K. Chan, and J. K. Nørskov, Understanding the apparent fractional charge of ions in the aqueous electrochemical double layer. **Nature Communications, 9**:3202 (2018) DOI: 10.1038/s41467-018-05511-y
14. R. B. Wexler, J. M. P. Martirez, and A. M. Rappe, Chemical Pressure-Driven Enhancement of the Hydrogen Evolving Activity of Ni_2P from Nonmetal Surface Doping Interpreted via Machine Learning. **Journal of the American Chemical Society*, 140,*** 4678-4683 (2018) DOI: 10.1021/jacs.8b00947
13. J. M. P. Martirez, and E. A. Carter, Prediction of a Low-Temperature N_2 Dissociation Catalyst Exploiting Near IR-to-Visible Light Nanoplasmonics. **Science Advances**, **3**, eaao4710 (2017) DOI: 10.1126/sciadv.aao4710

    - Featured in ***Chemical & Engineering News***: “Lowering the temperature on nitrogen splitting” by Sam Lemonick, January 3, 2018.
    - Princeton Engineering News: “New process could slash energy demands of fertilizer, nitrogen-based chemicals” by John Sullivan, January 12, 2018

12. R. B. Wexler, J. M. P. Martirez, and A. M. Rappe, Active Role of Phosphorus in the Hydrogen Evolving Activity of Nickel Phosphide (0001) Surfaces. **ACS Catalysis**, **7**, 7718-7725 (2017) DOI: 10.1021/acscatal.7b02761
11. J. M. P. Martirez, and E. A. Carter, Excited-State N_2 Dissociation Pathway on Fe-Functionalized Au. **Journal of the American Chemical Society**, **139**, 4390-4398 (2017) DOI: 10.1021/jacs.6b12301
10. D. F. Swearer, H. Zhao, L. Zhou, C. Zhang, H. Robatjazi, J. M. P. Martirez, C. M. Krauter, S. Yazdi, M. J. McClain, E. Ringe, E. A. Carter, P. Nordlander, N. J. Halas, Heterometallic Antenna-Reactor Complexes for Photocatalysis. **Proceedings of the National Academy of Sciences U.S.A., 113**, 8916-8920 (2016) DOI: 10.1073/pnas.1609769113
9. R. B. Wexler, J. M. P. Martirez, and A. M. Rappe, Stable Phosphorus Enriched (0001) Surfaces of Nickel Phosphides. **Chemistry of Materials, 28**, 5365-5372 (2016) DOI: 10.1021/acs.chemmater.6b01437
8. J. M. P. Martirez, and E. A. Carter, Thermodynamic Constraints in Using Au*M* (*M*= Fe, Co, Ni and Mo) Alloys as N_2 Dissociation Catalysts: Functionalizing a Plasmon-Active Metal. **ACS Nano, 10**, 2940-2949 (2016) DOI: 110.1021/acsnano.6b00085
7. Y. Qi, J. M. P. Martirez, W. A. Saidi, J.J. Urban, W.S. Yun, J.E. Spanier and A. M. Rappe, Modified Schottky emission to explain thickness dependence and slow depolarization in $BaTiO_3$ nanowires. **Physical Review B, 91**, 245431 (2015) DOI: 10.1103/PhysRevB.91.245431
6. J. M. P. Martirez, S. Kim, E. H. Morales, B. T. Diroll, M. Cargnello, T. R. Gordon, C. B. Murray, D. A. Bonnell, and A. M. Rappe, Synergistic Oxygen Evolving Activity of a TiO_2-rich Reconstructed $SrTiO_3$(001) Surface. **Journal of the American Chemical Society, 137**, 2939-2947 (2015) DOI: 10.1021/ja511332y

5. C. Baeumer, D. Saldana-Greco, J. M. P. Martirez, A. M. Rappe, M. Shim, and L. W. Martin, Ferroelectrically Driven Spatial Carrier Density Modulation in Graphene. **Nature Communications, 6**:6136 (2015) DOI: 10.1038/ncomms7136
4. W. A. Saidi*, J. M. P. Martirez*, and A. M. Rappe, Strong Reciprocal Interaction between Polarization and Surface Stoichiometry in Ferroelectric Oxides. **Nano Letters, 14**, 6711-6717 (2014) DOI: 10.1021/nl5035013
3. N. Koocher, J. M. P. Martirez, and A. M. Rappe, Theoretical Model of Oxidative Adsorption of Water on a Highly Reduced Reconstructed Oxide Surface. **Journal of Physical Chemistry Letters, 5**, 3408-3414 (2014) DOI: 10.1021/jz501635f
2. E. H. Morales*, J. M. P. Martirez*, W. A. Saidi, A. M. Rappe, and D. A. Bonnell, Coexisting Surface Phases and Coherent One-Dimensional Interfaces on $BaTiO_3$(001). **ACS Nano 8**, 4465-4473 (2014) DOI: 10.1021/nn501759g
1. J. M. P. Martirez, E. H. Morales, W. A. Saidi, D. A. Bonnell, and A. M. Rappe, Atomic and Electronic Structure of the $BaTiO_3$ (001) ($\sqrt{5}\times\sqrt{5}$) *R*26.6° Surface Reconstruction. **Physical Review Letters 109**, 256802 (1-5) (2012) DOI: 10.1103/PhysRevLett.109.256802

Students Mentored

Norleakvisoth Lim, *undergraduate*, University of California - LA, Fall 2019 - present
Alexander J. Tkalych, *graduate*, Princeton University, Fall 2017 – Spring 2018
Robert B. Wexler, *graduate*, University of Pennsylvania, Summer 2014 – Spring 2019
Joseph Abbate, *undergraduate*, Princeton University, Fall 2015 – Spring 2016
Nicole Belonzi, *graduate*, University of Pennsylvania, Summer 2014
Nathan Z. Koocher, *undergraduate*, University of Pennsylvania, Fall 2011 – Fall 2014

Recent Referee Services

Grant Proposal Review
Centro Svizzero di Calcolo Scientifico (CSCS, Swiss National Supercomputing Centre)

Scientific Article Review
ChemCatChem, Small, The Journal of Chemical Physics, Advanced Functional Materials, ACS Sustainable Chemistry & Engineering, ACS Nano, Nano Letters, ACS Catalysis, Nature Nanotechnology, The Journal of Physical Chemistry Letters, Angewandte Chemie

Most Recent Presentations (2017 – present)

Talks

7. ***Award talk*****:** "Accurate simulation of photochemical processes: From plasmon-driven photocatalysis to dye-sensitized photovoltaics" **ACS Fall 2020 Virtual Meeting & Expo** (August 19, 2020)
6. ***Invited seminar***: "Aiding in engineering new materials for sustainable energy applications: modelling ground- and excited-state catalysis on metals and metal oxides through the lens of accurate first-principles quantum mechanics", Department of Chemical Engineering, **Stanford University**, Stanford, California (March 20, 2019)
5. ***Invited:*** "Describing Light-Driven Catalysis on Surface-Doped Plasmonic Metals via Embedded Correlated Wavefunction Theories", **2018 MRS Fall Meeting and Exhibit**, Boston, Massachusetts, USA (November 27, 2018)
4. ***Invited*****:** "Ab initio modeling of light-driven catalysis on surface-doped plasmonic metals" **SciX 2018**, Atlanta, Georgia USA (October 24, 2018)

3. ***Invited*:** “Quantum mechanical description of excited-state catalysis on metals for nanoplasmonics” **255th American Chemical Society National Meeting and Exposition**, New Orleans, Louisiana USA (March 19, 2018)
2. ***Invited seminar***: “Surface phenomena on metals and metal oxides through the lens of first-principles quantum mechanics”, School of Chemical and Biomedical Engineering, **Nanyang Technological University, Singapore** (December 12, 2017)
1. “Quantum Mechanical Description of Excited-State Heterogeneous Catalysis Via Embedded Correlated Wavefunction Methods” **2017 American Institute of Chemical Engineers Annual Meeting**, Minneapolis, Minnesota, USA (October 31, 2017)

Posters

3. “Discovering and Understanding New Catalytic Materials for Sustainable Chemical Conversion via Quantum Mechanics” Princeton E-ffiliates Partnership 2018 Retreat, New York City, New York, USA (June 13, 2018)
2. “Understanding heterogeneous photochemical conversion processes from first principles” AFOSR 2018 Molecular Dynamics and Theoretical Chemistry Program Review, Albuquerque, New Mexico, USA (May 23, 2018)
1. “Excited-State Heterogeneous Catalysis on Surface-Doped Plasmonic Nanoparticles” *Gordon Research Conference* – Dynamics at Surfaces, Salve Regina University, Newport, RI, USA (July 30 - August 3, 2017)