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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
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Citation metrics (Google Scholar): 22 h-index
27 i10-index (1,758 total citations)

Education

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

B.S. in Chemistry (*Magna Cum Laude*), **2006**
University of Philippines, Diliman
Philippines

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 (September 2019 – present)
Supervisor: **Prof. Emily A. Carter** (Executive Vice Chancellor and Provost)
Department of Chemical and Biomolecular Engineering
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 grant applications
- participate in writing 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)
Department of Mechanical and Aerospace Engineering
Princeton University
Princeton, New Jersey, United States

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

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

39. A. Acosta, J. M. P. Martirez, N. Lim, J. P. Chang, and E. A. Carter, Influence of thickness and surface composition on the stability of ferroelectric polarization in HfO_2 thin films. **under review** (2022)
38. Q. Zhao, J. M. P. Martirez, and E. A. Carter, Charting C-C coupling pathways in electrochemical CO_2 reduction on Cu(111) using embedded correlated wavefunction theory. **under review** (2022)
37. L. Li, J. M. P. Martirez, and E. A. Carter, Identifying an Alternative Hydride Transfer Pathway for CO_2 Reduction on CdTe(111) and $CuInS_2$(112) Surfaces. **Advanced Theory and Simulations**, **5**, 2100413 (2022) DOI: 10.1002/adts.202100413
36. A. Acosta, J. M. P. Martirez, N. Lim, J. P. Chang, and E. A. Carter, Relationship between ferroelectric polarization and stoichiometry of HfO_2 surfaces. **Physical Review Materials**, **5**, 124417 (2021) DOI: 10.1103/PhysRevMaterials.5.124417

35. A. G. Rajan, J. M. P. Martirez, and E. A. Carter, The Coupled Effects of Temperature, Pressure, and pH on Water Oxidation Thermodynamics and Kinetics, **ACS Catalysis**, **11**, 11305-11319 (2021) DOI: 10.1021/acscatal.1c02428
34. J. M. P. Martirez and E. A. Carter, Metal-to-ligand-charge-transfer spectrum of a Ru-bipyridine-sensitized TiO_2 cluster from embedded multi-configurational excited-state theory, **Journal of Physical Chemistry A***,* **125**, 4998-5013 (2021) DOI: 10.1021/acs.jpca.1c02628
Part of "*125 Years of the Journal of Physical Chemistry*" special virtual issue
33. J. M. P. Martirez and E. A. Carter, Projector-free capped-fragment scheme within density functional embedding theory for covalent and ionic compounds, **Journal of Chemical Theory and Computation**, **17**, 4105-4121 (2021) DOI: 10.1021/acs.jctc.1c00285
32. L. Zhou, M. Lou, J. L. Bao, C. Zhang, J. G. Liu, J. M. P. Martirez, S. Tian, D. F. Swearer, H. Robatjazi, E. A. Carter, P. Nordlander, and N. J. Halas, Hot carrier multiplication in plasmonic photocatalysis, **Proceedings of the National Academy of Sciences U.S.A., 118**, e2022109118 (2021) DOI: 10.1073/pnas.2022109118
31. Q. Zhao, J. M. P. Martirez, and E. A. Carter, Revisiting understanding of electrochemical CO_2 reduction on Cu(111): competing proton-coupled electron transfer reaction mechanisms revealed by embedded correlated wavefunction theory. **Journal of the American Chemical Society**, **143**, 6152–6164 (2021) DOI: 10.1021/jacs.1c00880
30. *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**, **72,** 99-119 (2021) DOI: 10.1146/annurev-physchem-061020-053501
29. R. Sheil*, J. M. P. Martirez*, X. Sang, E. A. Carter, and J. P. Chang, Precise control of nanoscale Cu etching via gas-phase oxidation and chemical complexation. **Journal of Physical Chemistry C, 125**, 1819-1832 (2021) DOI: 10.1021/acs.jpcc.0c08932
Part of "*Emily A. Carter Festschrift*" special virtual issue
28. 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. **ACS Catalysis**, **10**, 12841-12857 (2020) DOI: 10.1021/acscatal.0c03140
27. 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). **Journal of Chemical Theory and Computation**, **16**, 7078–7088 (2020) DOI: 10.1021/acs.jctc.0c00341
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**, **10**, 11177-111234 (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 $p(2\times1)$ 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

Adrian Acosta, *graduate*, University of California, LA, Summer 2020 – present
Norleakvisoth Lim, *undergraduate*, University of California, LA, Fall 2019 – Summer 2020
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
Journal of Physical Chemistry C, 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)