Curriculum Vitae

JOHN MARK P. MARTIREZ

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Personal Information

Date of Birth	October 14, 1985
Birthplace	Tagbilaran city, Bohol, Philippines
Nationality	Filipino (US permanent resident)
Languages	English, Filipino

Professional Appointments

May 2018 – current	**Associate Research Scholar** *Advisor:* **Prof. Emily A. Carter** **Princeton University** Princeton, New Jersey, United States
March 2015 – April 2018	**Postdoctoral Research Associate** *Advisor:* **Prof. Emily A. Carter** **Princeton University** Princeton, New Jersey, United States
2006 – 2008	**University Instructor** University of the Philippines, Philippines

Education

2015	**Ph.D. in Chemistry** *Advisor*: **Prof. Andrew M. Rappe** **University of Pennsylvania** Philadelphia, Pennsylvania, United States
2006	**B.S. in Chemistry**, ***Magna cum Laude*** **University of the Philippines** - Diliman Diliman, Quezon City, Metro Manila, Philippines

Research Activities and Interests

I use state-of-the-art computational tools in fields where atomic-scale information delivers unparalleled chemical design principles. The main thrust of my work is using **first-principles density functional theory and embedded correlated wavefunction methods** to guide experimentalists in finding alternative and unconventional reaction pathways and catalysts for industrially relevant reactions. This includes computational investigations on manipulation of reactions via new or surface-modified heterogeneous catalysts and introduction of co-catalysts. The foundation of my work lay on the identification of key species and pathways in catalysis from first-principles quantum mechanics.

Patents

2. J. M. P. Martirez and E. A. Carter, Plasmonic Haber-Bosch catalysts based on surface-doped Au nanoparticles. ***Provisional 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 (* shared first authorship)

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. **submitted** (2018)
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. **under review** (2018)
18. A. J. Tkalych, J. M. P. Martirez, and E. A. Carter, Thermodynamic evaluation of trace-amount transition-metal ion doping in NiOOH films. **under review** (2018)
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**, **in press** (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**, **in press** (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, in press** (2018)
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.
- Featured in ***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

Alexander J. Tkalych, *graduate*, Princeton University, Fall 2017-present
Robert B. Wexler, *graduate*, University of Pennsylvania, Summer 2014-present (with ongoing mentoring and collaborations)
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 (while at Princeton)

Advanced Functional Materials, ACS Nano, Nano Letters, ACS Catalysis, Nature Nanotechnology, The Journal of Physical Chemistry Letters, Angewandte Chemie

Courses Taught

Undergraduate-level general, analytical, physical, and organic chemistry laboratory courses, University of the Philippines, Diliman, Philippines, 2006-2008

Presentations

Talks

13. ***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)
12. ***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)
11. "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)
10. "Plasmon-induced excited-state heterogeneous catalysis on surface-doped metallic nanoparticles" **253rd American Chemical Society National Meeting and Exposition**, San Francisco, California, USA (April 2017)
9. ***Invited*:** "Modeling Surface Phenomena via First-Principles Quantum Mechanics" **Center for Functional Nanomaterials, Brookhaven National Laboratory**, Upton, New York, USA (January 19, 2017)
8. ***Invited*:** "Excited-State Heterogeneous Catalysis on Metallic Nanoparticles" **2016 MRS Fall Meeting and Exhibit**, Boston, Massachusetts, USA (November 28 – December 2, 2016)
7. "Excited State Dissociation Pathway for N_2 on Fe-substituted Plasmon-Active Au" **AFOSR MURI Meeting**, Rice University, Houston, Texas, USA (May 2016)
6. ***Invited*:** "Role of charge-transfer excitations in Au-Fe alloys for heterogeneous N_2 dissociation catalysis" **251st American Chemical Society National Meeting and Exposition** (Computers in Chemistry), San Diego, California, USA (March 13-17, 2016)
5. "Dual active-site catalyst based on a single element for synergistic water-splitting", **9th International Workshop on Oxide Surfaces (IWOX- IX),** Granlibakken Conference Center, Tahoe City, California, USA (January 2014) *on behalf of Prof. Andrew M. Rappe*

4. "Thermodynamic and Kinetic Exploration of Surface Phase Coexistence on an Oxide Surface", **9th International Workshop on Oxide Surfaces (IWOX- IX)**, Granlibakken Conference Center, Tahoe City, California, USA (January 2014)
3. "Polarization Dependent Reconstructions of Ferroelectric Surfaces ", **APS March Meeting,** Boston, Massachusetts, USA (March 1, 2012)
2. "Hydration phase diagram for BaO terminated $BaTiO_3$", **APS March Meeting**, Dallas, Texas, USA (March 22, 2011)
1. "Theoretical study on the diffusion of hydroxyl radical on BaO terminated $BaTiO_3$(001) surface", **APS March Meeting,** Portland, Oregon, USA (March 18, 2010)

Posters

11. "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)
10. "Understanding heterogeneous photochemical conversion processes from first principles" AFOSR 2018 Molecular Dynamics and Theoretical Chemistry Program Review, Albuquerque, New Mexico, USA (May 23, 2018)
9. "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)
8. "Modeling Local Excited States on Surface Reactive Sites: An Exploration of Plasmon-Catalyzed CH_4 Dehydrogenation on Ru-functionalized Cu and N_2 Dissociation on Fe-functionalized Au" *AFOSR MURI Review Meeting*, Rice University, Houston, Texas, USA (December 7, 2016)
7. "Surface Functionalization of Plasmon-Active Au for Sustainable Ammonia Synthesis" *Andlinger Center Building Opening Celebration and Symposium*, Princeton University, Princeton, New Jersey, USA (May 2016)
6. "TiO-rich reconstructions of $BaTiO_3$(001) surface: The thermodynamics and kinetics of surface defect agglomeration leading to phase coexistence." *Dynamics, Interactions, and Electronic Transitions at Surfaces (DIET14 workshop)*, Pacific Grove, California, USA (October 2014)
5. "Synergistic Oxygen Evolving Activity of a Dual Active-site Catalysts Based on a Single Element", *Gordon Conference - Dynamics at Surfaces*, Salve-Regina University, Rhode Island, USA (August 2013)
4. "Strong Reciprocal Interaction between Polarization and Surface Stoichiometry in Ferroelectric Oxides*", International Workshop on Interfaces at Bear Creek*, Bear Creek Mountain Resort and Conference Center, Pennsylvania, USA (October 2012)
3. "Connection between relaxation of metastable polarization and time evolution of surface ion coverage in $BaTiO_3$ nanowires", *2011 Workshop on the Fundamental Physics of Ferroelectrics and Related Materials*, Gaithersburg, Maryland, USA (January 2011)
2. "First principle investigation of hydrogen transfer between surface adsorbed H_2O and OH on BaO (001) surface of thin film $BaTiO_3$", *ACS National meeting*, Boston, Massachusetts, USA (August 2010)
1. "First principles investigation of surface dynamics involving OH on thin-film $BaTiO_3$ surfaces", *22nd Annual Workshop on Electronic Structure Methods*, Austin, Texas, USA (June 2010)