## 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**

2015 – current	Postdoctoral Research Associate
	Advisor: Prof. Emily A. Carter
	Princeton University
	Princeton, New Jersey, United States
2006 - 2008	University Instructor
	Institute of Chemistry, University of the Philippines - Diliman

Diliman, Quezon City, Metro Manila, Philippines

#### **Education**

2015 **Ph.D. in Chemistry** 

Advisor: Prof. Andrew M. Rappe University of Pennsylvania

Philadelphia, Pennsylvania, United States **B.S. in Chemistry**, *Magna cum Laude* **University of the Philippines** - Diliman

Diliman, Quezon City, Metro Manila, Philippines

#### **Patent**

2006

1. <u>J. M. P. Martirez</u>, 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)

- 15. R. B. Wexler, <u>J. M. P. Martirez</u>, and A. M. Rappe, Chemical Pressure-Driven Enhancement of the Hydrogen Evolving Activity of Ni<sub>2</sub>P from Nonmetal Surface Doping Interpreted via Machine Learning. *submitted* (2018)
- 14. 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. *submitted* (2017)
- 13. J. M. P. Martirez, and E. A. Carter, Prediction of a Low-Temperature N<sub>2</sub> 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, <u>J. M. P. Martirez</u>, 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. <u>J. M. P. Martirez</u>, and E. A. Carter, Excited-State N<sub>2</sub> 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*, 113, 8916-8920 (2016) DOI: 10.1073/pnas.1609769113
- 9. R. B. Wexler, <u>J. M. P. Martirez</u>, 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. <u>J. M. P. Martirez</u>, and E. A. Carter, Thermodynamic Constraints in Using Au*M* (*M*= Fe, Co, Ni and Mo) Alloys as N<sub>2</sub> 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<sub>3</sub> nanowires. *Physical Review B*, 91, 245431 (2015) DOI: 10.1103/PhysRevB.91.245431
- 6. <u>J. M. P. Martirez</u>, 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<sub>2</sub>-rich Reconstructed SrTiO<sub>3</sub>(001) Surface. *Journal of the American Chemical Society*, 137, 2939-2947 (2015) DOI: 10.1021/ja511332y
- 5. C. Baeumer, D. Saldana-Greco, <u>J. M. P. Martirez</u>, 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, <u>J. M. P. Martirez</u>, 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\*, <u>J. M. P. Martirez\*</u>, W. A. Saidi, A. M. Rappe, and D. A. Bonnell, Coexisting Surface Phases and Coherent One-Dimensional Interfaces on BaTiO<sub>3</sub>(001). *ACS Nano* 8, 4465-4473 (2014) DOI: 10.1021/nn501759g
- 1. <u>J. M. P. Martirez</u>, E. H. Morales, W. A. Saidi, D. A. Bonnell, and A. M. Rappe, Atomic and Electronic Structure of the BaTiO<sub>3</sub> (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)

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**

- 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<sub>2</sub> 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<sub>2</sub> 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", 9<sup>th</sup>
  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", 9<sup>th</sup> 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<sub>3</sub>", **APS March Meeting**, Dallas, Texas, USA (March 22, 2011)
- 1. "Theoretical study on the diffusion of hydroxyl radical on BaO terminated BaTiO<sub>3</sub>(001) surface", **APS March Meeting,** Portland, Oregon, USA (March 18, 2010)

## **Posters**

- 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<sub>4</sub> Dehydrogenation on Ru-functionalized Cu and N<sub>2</sub> Dissociation on Fefunctionalized 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<sub>3</sub>(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<sub>3</sub> 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<sub>2</sub>O and OH on BaO (001) surface of thin film BaTiO<sub>3</sub>", *ACS National meeting*, Boston, Massachusetts, USA (August 2010)
- 1. "First principles investigation of surface dynamics involving OH on thin-film BaTiO<sub>3</sub> surfaces", *22nd Annual Workshop on Electronic Structure Methods*, Austin, Texas, USA (June 2010)