

Vitae

EMPLOYMENT

- 2007–Present: **Mount Holyoke College, MA**
Associate Professor of Chemistry.
- 2003–2007: **Mount Holyoke College, MA**
Assistant Professor of Chemistry.
- 1999–2003: **Vassar College, NY**
Assistant Professor of Chemistry.
- 1997–1999: **Los Alamos National Laboratories, NM**
Postdoctoral research with Lawrence R. Pratt.

EDUCATION

- 1992–1997: **Brown University**
Doctor of Philosophy, Theoretical Chemistry (supervisor Jimmie D. Doll).
“*Structure and Dynamics of Adsorbates on Metal Surface Systems.*”
Honors and Awards: AT&T Bell Laboratories CRFP Fellow (1992-7); NSF Fellow (1992-4); Gordon Research Conference on "Dynamics at Surfaces" Scholarship (1995); NSF Travel Award to Enrico Fermi School of Physics Course 79 (1994); NATO ASI Scholarship to Enrico Fermi School of Physics Course 79 (1994); Accounts of Chemical Research Departmental Graduate Prize (1993)
- 1988–1992: **Rhode Island College**
Bachelor of Arts (BA), Chemistry, Physics, Applied Mathematics, *Summa Cum Laude*
Chemistry Honors Thesis: Excited-State Acid-Base Properties of Trisbipyrazine Ruthenium (II)
Mathematics Honors: Advanced work in real analysis and ordinary differential equations.
Honors and Awards: Eleanor M. McMahon Award (Honors program Award) (1992); Christopher R. Mitchell Award (Departmental Mathematics Award) (1992); Departmental Physics Award (1992); Ronald J. Boruch Award (Physical Sciences Award) (1992); Eastern Colleges Science Conference – Outstanding Chemistry paper (1991); American Chemical Society Undergraduate Departmental Award (1991); National Hispanic Scholarship Foundation Scholar (1990); Kraft General Foods Scholar (1989); CRC Press Freshman Chemistry Award (1989)

COURSES TAUGHT

- General Chemistry I and II
- Chemical Thermodynamics
- Atomic and Molecular Structure
- Simulating Chemistry, Biochemistry, and Materials Science

- Ceramics
- Using Spectroscopy to Analyze Paintings

PUBLICATIONS

(*undergraduate co-authors)

1. F. G. Haibach, M. A. Gomez, E. Fitzgerald, K. E. Paczkowski*, "NIR imaging of paintings: Looking for deeper meaning," *Chemical Educator*, **12**, 349 (2007).
2. M. A. Gomez, Saryu Jindal*, Katharyn M. Fletcher*, Leigh S. Foster*, Nanna Dufie A Addo*, Debbie Valentin*, Cristina Ghenoiu*, and Abigail Hamilton*, "A comparison of proton conduction in KTaO_3 and SrZrO_3 ," *J. Chem. Phys.* **126**, 194701 (2007)
3. M. A. Gomez, L. R. Pratt, J. D. Kress, and D. Asthagiri, "Water adsorption and dissociation on BeO (001) and (100) surfaces," *Surface Science*, **601**, 1608 (2007).
4. M. A. Gomez, and P. Peart*, "Including quantum subsystem character within classical equilibrium simulations," *J. Chem. Phys.* **125**, 034105 (2006).
5. M. A. Gomez, M. A. Griffin*, S. Jindal*, K. D. Rule*, and V. Cooper*, "The effect of octahedral tilting on proton binding sites and transition states in pseudo-cubic perovskite oxides," *J. Chem. Phys.* **123**, 094703 (2005).
6. D. Asthagiri, L. R. Pratt, J. D. Kress, and M. A. Gomez, "Hydration and mobility of HO^+ (aq)," *Proc. Natl. Acad. Sci. USA* **101**, 7229 (2004).
7. D. Asthagiri, L. R. Pratt, J. D. Kress, and M. A. Gomez, "The hydration state of HO^+ ," *Chemical Physics Letters* **380**, 530 (2003).
8. P. Grabowski*, D. Riccardi*, M. A. Gomez, D. Asthagiri, and L. R. Pratt, "Quasi-chemical theory and the standard free energy of H^+ (aq)," *J. Phys. Chem. A.* **106**, 9145 (2002).
9. L. R. Pratt, R. A. LaViolette, M. A. Gomez, and M. E. Gentile*, "Quasi-chemical Theory for the Statistical Thermodynamics of the Hard Sphere Fluid." *J. Phys. Chem. B.* **105**, 11662 (2001).
10. B. S. Jorgensen, R. C. Dye, L. R. Pratt, M. A. Gomez, J. E. Meadows, "Concentrating Low Level Tritiated Water Through Isotope Exchange." *Fusion Technology* **37**, 124 (2000).
11. M. A. Gomez, L. R. Pratt, G. Hummer, and S. Garde, "Default Models for Information Theories of Hydrophobic Effects," *J. Phys.Chem.*, **103**, 3520 (1999).
12. M. A. Gomez and L. R. Pratt, "Construction of Simulation Wave Functions for Aqueous Species: D_3O^+ ," *J. Chem. Phys.* **109**, 8783 (1998).
13. J. T. Kindt, J. C. Tully, M. Head-Gordon, and M. A. Gomez, "Electron-hole Pair Contributions to Scattering, Sticking, and Surface Diffusion: CO on $\text{Cu}(100)$," *J. Chem. Phys.* **109**, 3629 (1998).
14. M. A. Gomez, B. Chen, J. D. Doll, and D. L. Freeman "Quantum Mechanics of Hydrogen on Nickel and Palladium Clusters" in Theory of Atomic and Molecular Clusters, J. Jellinek, ed. (Springer-Verlag, Berlin, 1998).

15. B. Chen, M. A. Gomez, J. D. Doll, and D. L. Freeman, "Theoretical Studies of the Effect of Hydrogen-Hydrogen Interactions on the Structural and Dynamical Properties of Metal/Hydrogen Clusters," *J. Chem. Phys.* **108**, 4031 (1998).
16. B. Chen, M. A. Gomez, M. Sehl, J. D. Doll, D. L. Freeman. "Diffusion and Path Integral Monte Carlo Investigations of Nickel and Palladium Clusters." *J. Chem. Phys.* **105**, 9686 (1996).
17. B. Finnilla, M. A. Gomez, C. Sebenik, C. Stenson, and J. D. Doll. "Quantum annealing: a new method for minimizing multidimensional functions." *Chem. Phys. Lett.* **219**, 343-348 (1994).
18. J. C. Tully, M. Gomez, and M. Head-Gordon. "Electronic and phonon mechanisms of vibrational relaxation: CO on Cu(100)" *J. Vac. Sci. Technol. A* **11**, 1914 (1993).
19. D. L. Lynch, S. W. Rick, M. A. Gomez, B. W. Spath, J. D. Doll, and L. R. Pratt. "Spectroscopic studies of surface and subsurface hydrogen/metal systems" *J. Chem. Phys.* **97**, 5177 (1992).

RESEARCH FUNDING, 1999–present

Total: \$1,430,581

Henry Dreyfus Teacher-Scholar Award (2007-2012), \$60,000

Maria A. Gomez

"The elusive proton: Finding conduction pathways in solid and liquid phases" (5 year award)

National Science Foundation—RUI (2006-2010), \$185,000

Maria A. Gomez

"Understanding how dopant affects preferred proton conduction pathways in perovskite oxides"
Award Number: CHE-0608813 (4 year award separated into 2 two year awards)

Petroleum Research Fund – Type B (2006–2009), \$50,000

Maria A. Gomez

"Thermodynamic and kinetic studies of hydrogen isotope binding on selective materials."

National Science Foundation – MRI (2005–2008), \$100,000

George Shields, Maria A. Gomez, Carol Parish, Marc Zimmer, Maria Nagan, Tricia Sheperd, Glênisson de Oliveira, and Wingfield Glassey

"Acquisition of a linux cluster for the Molecular Education and Research Consortium in Undergraduate computational chemistRY (MERCURY)" Award Number: CHE-052063.

National Science Foundation—NUE (2004–2006), \$100,000

Sean Decatur, Donald Cotter, Wei Chen, Maria A. Gomez, Darren Hamilton, Megan Nuñez

"NUE: Integration of nanotechnology into the core chemistry curriculum at Mount Holyoke College" Award Number: 0407117.

Petroleum Research Fund – Type G (2003–2006), \$35,000

Maria A. Gomez

"Proton conduction in perovskite oxides."

National Science Foundation – MRI (2003–2005), \$780,200

George Shields, Jeffery Greathouse, Maria A. Gomez, Carol Parish, Ramona Taylor, Martha Reynolds, and Marc Zimmer

"Acquisition of high performance computers for the northeastern undergraduate research chemistry consortium" Award Number: CHE-0116435.

National Science Foundation – MRI (2000–2002), \$100,381

Bradley E. Richards, Maria A. Gomez, James C. Lombardi

"Acquisition of an 8-processor Sun" Award Number: EIA-0079466.

Camille and Henry Dreyfus Faculty Start-Up Grant for Undergraduate Institutions (1999–2004), \$20,000

Maria A. Gomez

"The quantum mechanics of proton transfer."

PROFESSIONAL ORGANIZATIONS & ACTIVITIES

MERCURY Member – We organize an annual national conference on computational chemistry specially designed for undergraduates. See <http://mars.chem.hamilton.edu/> for details.

American Chemical Society member

American Physical Society member

Sigma Xi member

Reviewer, NSF, DOE, PRF

Panel member, NSF 2005, 2006, 2007

Reviewer, Journal of Chemical Physics, Journal of Physical Chemistry, Chemistry of Materials, Journal of Chemical Education