Awards

- ISCRE 24 Dow travel award (2016)
- University of Delaware Graduate Student of Distinction (2015)
- Meritorious recognition in the Mathematical Contest in Modeling (2010)
- Top 500 Nationwide in the William Lowell Putnam Mathematical Competition (2010)

Software Contributions

CoolVent coolvent.mit.edu

Natural ventilation simulation tool for designing buildings

- Developed the graphical user interface

MSA-KMC dion.che.udel.edu/downloads

Multiscale KMC code with built-in sensitivity analysis

- Developed from scratch

Zacros dion.che.udel.edu/downloads

Graph-theoretical KMC software

- Implemented a sensitivity analysis module

Publications

- **M.P. Nunez**, D.K. Zerkle, J.M. Zucker, "The rheology of molten Composition B" Los Alamos National Lab Report LA-UR-12-24029 (2012).
- D. K. Zerkle, **M. P. Núñez**, and J. M. Zucker, "Molten Composition B Viscosity at Elevated Temperature" Journal of Energetic Materials 34(4), 368 (2016).
- **M. Núñez** and D.G. Vlachos, "Steady state likelihood ratio sensitivity analysis for stiff kinetic Monte Carlo simulations" Journal of Chemical Physics 142(4), 044108 (2015).
- A. Hashemi, **M. Núñez**, P. Plechac, D.G. Vlachos, "Stochastic Averaging and Sensitivity Analysis for Two Scale Reaction Networks" Journal of Chemical Physics 144, 074104 (2016).
- **M. Núñez** and D.G Vlachos, "Surface engineering of catalyst facet structure and its application to the oxygen reduction reaction" Nature Chemistry (submitted)
- S. Dutta, A. Bohre, G.R. Jenness, W. Zheng, **M. Núñez**, D.G. Vlachos, B. Saha, "Improved Graphene Oxide for Efficient Solventless C-C Coupling of Low Carbon Furanics to High Carbon Fuel Precursors" ACS Catalysis (submitted)
- **M. Núñez**, T.A. Robie, and D.G Vlachos, "Rapid identification of the rate determining step in complex kinetic systems" (in preparation)

Selected Presentations

Poster

- M. Nunez and D.G. Vlachos, "Condition-Dependent Structure Sensitivity of CO Oxidation" Center for Catalytic Science and Technology Annual Research Review, Newark, DE, Sep. 23, 2013.
- M. Nunez and D.G. Vlachos, "First Principles Prediction of Active Sites for Transition Metal Catalysts" Center for Catalytic Science and Technology Annual Research Review, Newark, DE, Oct. 8, 2015.
- M. Nunez and D.G. Vlachos, "Identification of Active Sites On Transition Metal Catalysts" 24th International Symposium on Chemical Reaction Engineering, Minneapolis, MN, Jun. 13, 2016.

Oral

- M. Nunez and D.G. Vlachos, "Uncertainty Quantification in Stochastic Multiscale Models of Heterogeneous Catalysis" American Institute of Chemical Engineers Annual Meeting, Atlanta, GA, Nov. 18, 2014.
- M. Nunez and D.G. Vlachos, "Designing Active Sites from First Principles" American Institute of Chemical Engineers Annual Meeting, Salt Lake City, UT, Nov. 12, 2015.
- M. Nunez and D.G Vlachos, "Optimization of Transition Metal Catalyst Structure for the Oxygen Reduction Reaction" 252nd American Chemical Society National Meeting & Exposition, Philadelphia, PA, Aug. 22, 2016.