

## Investigator's Experience and Competence

- PI of the Office of Basic Energy Science, Department of Energy (BES/DOE) Physical Biosciences Program at PNNL. The program is focused on uniquely characterizing the critical biochemical and biophysical features of enzymatic processes related to producing a suite of small sustainable energy carriers.
- Thrust Lead for Theory and Computation for the Center for Molecular Electrocatalysis, an Energy Frontier Research Center focusing on understanding proton and electron transfer processes in electrocatalytic systems.
- Co-PI of BES/DOE Catalysis Program at PNNL. The program focuses on advancing the design of catalysts with improved performances for a carbon-neutral energy future via a qualitative and quantitative mechanistic molecular-level understanding of reaction pathways.



## Education and Training

University of Florence, Italy

Bachelor in Chemistry, 1996

University of Florence, Italy

Ph.D., 2000

Max Planck Institute for Solid State Physics, Stuttgart, Germany  
Detached study from Ph. D. program

1997-1998

University of Pennsylvania

Postdoctoral Fellow, 2000-2002

## Research and Professional Experience

Chief Scientist, Pacific Northwest National Laboratory, WA (2015-present)

Research Professor, Washington State University, WA (2017-present)

Visiting Professor, University of Montpellier 2, France (2014)

Adjunct Professor in Biophysics, German Research School for Simulation Sciences, Germany (2011-present)

Senior Scientist, Pacific Northwest National Laboratory, WA (2010-2014)

Assistant Professor, International School for Advanced Studies, Italy (2002-2009)

## Awards

Exceptional Scientific Achievement Award, Pacific Northwest National Laboratory (2019)

Laboratory Director's Path to Excellence Award, Pacific Northwest National Laboratory (2016)

2015 ACS Catalysis Lectureship for the Advancement of Catalytic Science (2015)

## Selected Recent Publications (10 out of 130)

1. B. Ginovska, O. Y. Gutiérrez, A. Karkamkar, M.-S. Lee, J. Lercher, Y. Liu, S. Raugei, R. Rousseau, W. J. Shaw. Bioinspired Catalyst Design Principles: Progress in Emulating Properties of Enzymes in Synthetic Catalysts. *ACS Catalysis* **13** (2023) 11883.
2. D. A. Lukoyanov, Z.-Y. Yang, A. Pérez-González, S. Raugei, D. R. Dean, L. C. Seefeldt, B. M. Hoffman. <sup>13</sup>C ENDOR Characterization of the Central Carbon within the Nitrogenase Catalytic Cofactor Indicates That the CFe6 Core Is a Stabilizing "Heart of Steel". *J. Am. Chem. Soc.* **144** (2022) 18315.
3. E. S. Wiedner, A. M. Appel, S. Raugei, W. J. Shaw, R. M. Bullock, Molecular Catalysts with Diphosphine Ligands Containing Pendant Amines. *Chem. Rev.* **122** (2022) 12427.
4. A. Patwardhan, R. Sarangi, B. Ginovska, S. Raugei, S. W. Ragsdale. Nickel–Sulfonate Mode of Substrate Binding for Forward and Reverse Reactions of Methyl–SCoM Reductase Suggests a Radical Mechanism Involving Long-Range Electron Transfer. *J. Am. Chem. Soc.* **143** (2021) 5481.
5. J. H. Art, O. A. Zadornyy, D. W. Mulder, S. M. Keable, A. E. Cohen, M. W. Ratzloff, S. G. Williams, B. Ginovska, N. Kumar, J. Song, S. E. McPhillips, C. M. Davidson, A. Y. Lyubimov, N. Pence, G. J. Schut, A. K. Jones, S. M. Soltis, M. W. W. Adams, S. Raugei, P. W. King, J. W. Peters. *Tuning catalytic bias of hydrogen gas producing hydrogenases.* *J. Am. Chem. Soc.* **141** (2020) 1227.
6. L. C. Seefeldt, Z.-Y. Yang, D. A. Lukoyanov, D. F. Harris, D. R. Dean, S. Raugei, B. M. Hoffman. *Reduction of*

Substrates by Nitrogenases. Chem. Rev. **120** (2020) 5082.

7. V. Hoeke, L. Tociu, D. A. Case, L. C. Seefeldt, S. Raugei, B. M. Hoffman. High resolution ENDOR spectroscopy combined with quantum chemical calculations reveals the structure of the nitrogenase Janus intermediate E<sub>4</sub>(4H). J. Am. Chem. Soc. **141** (2019) 11984. Erratum: J. Am. Chem. Soc. **141** (2019) 19950.
8. S. Raugei, L. C. Seefeldt, and B. H. Hoffman. A Critical Computational Analysis Illuminates the Reductive-Elimination Mechanism That Activates Nitrogenase for N<sub>2</sub> Reduction. Proc. Nat. Acad. Sci. **115** (2018) E10521.
9. N. Khadka, R. D. Milton, S. Shaw, D. Lukoyanov, D. R. Dean, S. D. Minter, S. Raugei, B. M. Hoffman, L. C. Seefeldt. Mechanism of Nitrogenase H<sub>2</sub> Formation by Metal-Hydride Protonation Probed by Mediated Electrocatalysis and H/D Isotope Effects. J. Am. Chem. Soc., **139**, 13518 (2017).
10. T. Wongnate, D. Sliwa, B. Ginovska, D. Smith, M. W. Wolf, N. Lehnert, S. Raugei, S. W. Ragsdale. The radical mechanism of biological methane synthesis by methyl- coenzyme M reductase. Science, **352**, 953 (2016).

### **Synergistic Activities**

- Organizer: of the symposium on New Paradigm for Catalyst Design: From Enzymatic Function to Functional Mimics, 254<sup>th</sup> ACS National Meeting, Washington, DC, August 21-22, 2017.
- Organizer: Workshop on “Material Science for Energy Storage”, International Centre for Theoretical Physics, Trieste (Italy), to be held on May 11-15, 2015.
- Organizer: Conference on “Progress in Ab Initio Modelling of Biomolecules: Towards computational spectroscopy,” University “La Sapienza,” Rome (Italy), April 2-4, 2007.
- Organizer: Workshop “Ab initio modeling in biological systems,” International School for Advanced Studies, Trieste (Italy), May 15-16, 2004.
- Panelist for the Office of Basic Energy Science, Department of Energy of the United States, the National Science Foundation of the United States, European Research Council (ERC), and the Partnership for Advanced Computing in Europe (PRACE).