Nitish Govindarajan

PhD Candidate

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Research Interests

Electrocatalysis, reaction mechanisms, density functional theory, molecular dynamics, enhanced sampling, solvent effects, molecular catalysts, electrode-electrolyte interfaces, activity descriptors

Education

2016–2020 **Ph. D.**, *Chemistry*, University of Amsterdam, The Netherlands.
Advisor: Prof. Evert Jan Meijer

2013–2014 **M. S.**, *Chemical Engineering*, Carnegie Mellon University, USA.
Advisor: Prof. John Kitchin

2009–2013 **B. Tech.**, *Chemical Engineering*, SASTRA University, India.
GPA: 9.08/10.0, First class with distinction

Research Experience

02/16–Present **Ph. D. Candidate**, *Van 't Hoff Institute for Molecular Science*, University of Amsterdam, The Netherlands.
Thesis topic: Modeling solvent effects in catalytic reactions for energy conversion.

07/19–08/19 **Visiting Researcher**, *Department of Chemistry*, University of Cambridge, UK.
Project topic: Understanding the effect of the electrical double layer on the TiO_2-electrolyte interface using *ab-initio* molecular dynamics and finite field methods. Advisor: Prof. Michiel Sprik.

05/18–07/18 **HPC Europa Visiting Researcher**, *IQTCUB*, University of Barcelona, Spain.
Project topic: Descriptor based analyses and solvent effects on activity predictions and pathway bifurcation in electrocatalytic reactions. Advisor: Dr. Federico Calle-Vallejo

11/17–12/17 **Visiting Researcher**, *Chair for Theoretical Chemistry*, Technical University Munich, Germany.
Project topic: Understanding the role of defects for oxygen evolution on the Anatase TiO_2-water interface using ab-initio molecular dynamics. Advisors: Dr. Harald Oberhofer and Prof. Karsten Reuter

12/13–12/14 **Graduate Researcher**, *Department of Chemical Engineering*, Carnegie Mellon University, USA.
Thesis topic: Modeling pervoskites for thermochemical CO_2/H_2O conversion using density functional theory and ab-initio thermodynamics.

03/13–06/13 **Student Research Assistant**, *Institute of Technical Physics*, KIT, Germany.
Thesis topic: Investigation of Fibre-Bragg grating based flow sensors for cryogenic applications.

Professional Experience

09/15–02/16 **Process Engineer**, *Bloom Energy*, Sunnyvale, CA, USA.
Job responsibilities: Data processing/analysis to optimize operation of energy servers, development of user interfaces for quick analysis by the operations team.

01/15–07/15 **Controls Engineering Intern**, *Bloom Energy*, Sunnyvale, CA, USA.
Job responsibilities: Development of algorithms for control automation of energy servers.

Publications († = Equal Contribution)

9 **On the dynamic nature of ligand pK_a during homogeneously catalyzed aqueous methanol dehydrogenation**, *N. Govindarajan, H. Beks, and E. J. Meijer, To be submitted*, (2020).

8 **An In-Depth Mechanistic Study of Ru Catalysed Aqueous Methanol Dehydrogenation and Prospects for Future Catalyst Design**, *N. Govindarajan†, V. Sinha†, M. Trincado, H. Grützmacher, E. J. Meijer, and B. de Bruin, ChemRxiv*, (2019).

7 **Elucidating Cation Effects in Homogeneously Catalyzed Formic Acid Dehydrogenation**, *N. Govindarajan and E. J. Meijer, Faraday Discuss.*, 220, 404 (2019).

6 **Selective surface functionalization generating site-isolated Ir on MnOx/N-doped carbon composite for robust electrocatalytic water oxidation**, *N. Yan, R. Detz, N. Govindarajan, J. M. Koelewijn, B. Hua, P. Li, E. J. Meijer, and J. N. H. Reek, J. Mater. Chem. A*, 7, 23098 (2019).

5 **Modeling the Catalyst Activation Step in a Metal-Ligand Radical Mechanism Based Water Oxidation System**, *N. Govindarajan and E. J. Meijer, Inorganics*, 7, 62 (2019).

4 **Outlining the Scaling-based and Scaling-free Optimization of Electrocatalysts**, *N. Govindarajan, M. T. M. Koper, E. J. Meijer, and F. Calle-Vallejo, ACS Catal.*, 9, 4218 (2019).

3 **How Solvent Affects C-H activation and Hydrogen Production Pathways in Homogeneous Ru-catalyzed Methanol Dehydrogenation Reactions**, *V. Sinha†, N. Govindarajan†, B. de Bruin, and E. J. Meijer, ACS Catal.*, 8, 6908 (2018).

2 **Impact of the Ligand Flexibility and Solvent on the O-O bond formation step in a highly active Ru Water Oxidation catalyst**, *N. Govindarajan, A. Tiwari, B. Ensing, and E. J. Meijer, Inorg. Chem.*, 57, 13063 (2018).
ACS Editors' Choice, Front Cover Article

1 **Does the breaking of adsorption-energy scaling relations guarantee enhanced electrocatalysis?**, *N. Govindarajan, J. M. Garcia-Lastra, E. J. Meijer, and F. Calle-Vallejo, Curr. Opin. Electrochem*, 8, 110 (2018).

Selected Talks

2019 **Importance of ligand acidity constants in homogeneously catalyzed methanol dehydrogenation**, *HRSMC Lustrum Symposium, Amsterdam, The Netherlands.*

2019 **Modeling solvent effects in catalytic reactions for energy conversion**, *North American Catalysis Society Meeting (NAM26), Chicago, USA.*

2018 **Realistic modeling of homogeneously catalyzed dehydrogenation reactions**, *CHAINS, The Dutch Chemistry Conference, Veldhoven, The Netherlands*.

2017 **Effect of solvent on Ru catalyzed methanol dehydrogenation**, *Future Energy Conference, Eindhoven, The Netherlands*.

2017 **Modeling solvent effects in catalysis for energy conversion**, *Frontiers of Multiscale Modeling in Materials, Energy & Catalysis III, Heilinghenhafen, Germany*.

2017 **Understanding aqueous proton transfer in ruthenium catalyzed water splitting**, *Netherlands Chemistry and Catalysis Conference (NCCC XXII), Noordwijkerhout, The Netherlands*.

Awards & Honors

2018 **HPC-Europa3 visitor fellowship**, *Visitor fellowship and grant for supercomputer time in MareNostrum at the Barcelona Supercomputing Center (BSC)*.

2015 **Shell-CSER PhD fellowship**, *Selected as a part of the 'Computational Sciences for Energy Research' initiative from a pool of 1500 candidates*.

2013 **Semester abroad scholarship**, *Scholarship for a research visit to KIT, Germany for undergraduate thesis project*.

2010, 2011, & 2012 **Dean's merit list**, *awarded to top 10 % of all undergraduates*.

Teaching

2018, 2019 **Teaching assistant**, *5112KATA6Y: Catalysis*, Developed a hands-on exercise on computational eletrocatalysis.

2016, 2017, & 2018 **Teaching assistant**, *5112QUAN6Y: Quantum Chemistry*, Assisted undergraduate students on exercises and assignments.

2018, 2019 **Teaching assistant**, *Molsim: CECAM Winter School*, Assisted participants on exercise sessions.

Mentoring

2019 **Master research thesis**, *Hugo Beks*, Determining acidity constants from DFT based molecular dynamics.

2018 **Master literature thesis**, *Tobias Verdonschot*, Modeling metal oxides using DFT.

2016, 2017 **Undergraduate student projects**, *Supervised 4 students on one month projects*.

Skills

Python, LaTeX, Shellscript, Emacs, Javascript, HTML, CP2K, VASP, VMD

Service

Referee: Journal of Catalysis