

# Nitish Govindarajan

Postdoctoral Researcher

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## Research Interests

Computational electrocatalysis, catalytic reaction mechanisms, density functional theory (DFT), DFT based molecular dynamics, enhanced sampling, solvent effects, molecular catalysts, electrode-electrolyte interfaces, catalytic activity descriptors

## Education

- 2016–2020 **Ph. D.**, *Chemistry*, University of Amsterdam, The Netherlands.  
Thesis: [Modeling solvent effects in catalytic reactions for energy conversion](#). Promoter: Prof. Evert Jan Meijer. Co-Promoter: Prof. Peter Bolhuis
- 2013–2014 **M. S.**, *Chemical Engineering*, Carnegie Mellon University, USA.  
Thesis: Modeling pervoskites for thermochemical CO<sub>2</sub>/H<sub>2</sub>O conversion using density functional theory and ab-initio thermodynamics. Advisor: Prof. John Kitchin
- 2009–2013 **B. Tech.**, *Chemical Engineering*, SASTRA University, India.  
First class with distinction (GPA: 9.1/10)

## 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.

## Research Experience

- 05/20–  
Present **Postdoctoral Researcher**, *Catalysis Theory Center*, DTU, Denmark.  
Understanding electrocatalytic reaction mechanisms and solvent effects in electrode-electrolyte interfaces. Advisor: Prof. Karen Chan
- 02/16–03/20 **Ph. D. Candidate**, *Van 't Hoff Institute for Molecular Science*, University of Amsterdam, The Netherlands.  
Used first principles based molecular dynamics simulations and advanced sampling methods to understand catalytic reactions in complex environments.
- 07/19–08/19 **Visiting Researcher**, *Department of Chemistry*, University of Cambridge, UK.  
Worked on understanding the effect of the electrical double layer on the TiO<sub>2</sub>-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.  
Developing descriptor based analysis for electrocatalyst screening studies. Advisor: Dr. Federico Calle-Vallejo

- 11/17–12/17 **Visiting Researcher**, *Chair for Theoretical Chemistry*, Technical University Munich, Germany.  
Used ab-initio molecular dynamics simulations to understand the role of defects for oxygen evolution on the Anatase TiO<sub>2</sub>-water interface. Advisors: Dr. Harald Oberhofer and Prof. Karsten Reuter
- 12/13–12/14 **Graduate Researcher**, *Department of Chemical Engineering*, Carnegie Mellon University, USA.  
Used DFT and ab-initio thermodynamics to predict oxygen vacancy concentrations in perovskites for thermochemical H<sub>2</sub>O conversion. Advisor: Prof. John Kitchin
- 03/13–06/13 **Student Research Assistant**, *Institute of Technical Physics*, KIT, Germany.  
Performed simulations and experiments to investigate Fibre-Bragg grating based flow sensors for cryogenic applications as a part of my undergraduate thesis project.

### Publications: First Author († = Equal Contribution)

- 8 **Variability of ligand pK<sub>a</sub> during homogeneously catalyzed aqueous methanol dehydrogenation**, *N. Govindarajan, H. Beks, and E. J. Meijer, ACS Catal.*, 10, 14775 (2020).
- 7 **An In-Depth Mechanistic Study of Ru Catalysed Aqueous Methanol Dehydrogenation and Prospects for Future Catalyst Design**, *N. Govindarajan<sup>†</sup>, V. Sinha<sup>†</sup>, M. Trincado, H. Grützmacher, E. J. Meijer, and B. de Bruin, ChemCatChem*, 20, 12 (2020).
- 6 **Elucidating Cation Effects in Homogeneously Catalyzed Formic Acid Dehydrogenation**, *N. Govindarajan and E. J. Meijer, Faraday Discuss.*, 220, 404 (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<sup>†</sup>, N. Govindarajan<sup>†</sup>, B. de Bruin, and E. J. Meijer, ACS Catal.*, 8, 6908 (2018).  
**Corresponding author**
- 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).

### Publications: Contributing Author

- 2 **Effect of monomer precursors with identical functionality on the properties of the physical network**, *A. Torres-Knopp, V. Schamboeck, N. Govindarajan, P. D. Iedema, and I. Kryven, Communications Materials, Accepted*, (2021).

- 1 **Selective surface functionalization generating site-isolated Ir on MnO<sub>x</sub>/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).

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

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## Awards & Honors

- 2021 **PRACE Project Access**, Co-applicant for the project "Computational electrocatalysis for a sustainable carbon cycle" that was awarded 37 million CPU hrs as a part of the PRACE 22nd call for project access.
- 2021 **MSCA Seal of Excellence**, For securing > 85 % for the MSCA Individual Fellowship proposal on Multiscale modeling of nanostructured Cu electrodes for CO<sub>2</sub> reduction.
- 2018 **HPC-Europa3 visitor fellowship**, Visitor fellowship and grant for supercomputer time in MareNostrum at the Barcelona Supercomputing Center (BSC).
- 2015 **Shell-NWO 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 my undergraduate thesis project.
- 2010, 2011, & 2012 **Dean's merit list**, awarded to top 10 % of all undergraduates.

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## Teaching

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

- 2020 **PhD thesis**, *Sihang Liu*, Topic: Computational electrocatalysis for biomass conversion.
- 2019 **Master research thesis**, *Hugo Beks*, Topic: Determining acidity constants from DFT based molecular dynamics.
- 2018 **Master literature thesis**, *Tobias Verdonschot*, Topic: Modeling metal oxides using DFT.
- 2016, 2017 **Undergraduate student projects**, *Supervised 4 second year Bachelor students on one month projects.*

## Skills

Python,  $\text{\LaTeX}$ , Shellsript, Emacs, Javascript, HTML, CP2K, GPAW, VASP, VMD

## Service and Outreach

- 2020 Co-organizer of Catalysis in the time of Coronavirus: An online webinar series
- 2019-Present Referee: Journal of Catalysis, ACS Applied Materials & Interfaces, ACS Catalysis
- 2016-2018 Editorial board: Amsterdam Science Magazine