Nitish Govindarajan

Postdoctoral Researcher

DTU Physics, Fysikvej 307
Kgs. Lyngby, Denmark
✉ *gnitish.1991@gmail.com*
nitish_gov
nitishg91

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, microkinetic modeling

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_2/H_2O conversion using density functional theory and ab-initio thermodynamics. Advisor: Prof. John Kitchin

2009–2013 **B. Tech.**, *Chemical Engineering*, SASTRA University, India.
Thesis: Investigation of Fibre-Bragg grating based flow sensors for cryogenic applications, 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 electrolyte effects at solid-liquid interfaces using constant potential DFT methods, molecular dynamics and microkinetic modeling.

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_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.
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_2-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-inito thermodynamics to predict oxygen vacancy concentrations in perovskites for thermochemical H_2O conversion. Advisor: Prof. John Kitchin

03/13–06/13 **Student Research Assistant**, *Institute of Technical Physics*, KIT, Germany.
Peformed 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)

Citation Metrics (Google Scholar): h-index: 6, Total citations: 162 (04/2021)

10 **Improving the intrinsic activity of electrocatalysts for sustainable energy conversion: where are we and where can we go?**, *N. Govindarajan, G. Kastlunger, H. H. Heenen, and K. Chan*, In preparation, (2021).

9 **On the differences in alkaline CO electro-oxidation on Copper and Gold Single Crystals**, *A. Tiwari†, N. Govindarajan†, H. Heenen, A. S. Bjorlund, K. Chan and S. Horch*, In preparation, (2021).

8 **Variability of ligand pK_a 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†, V. Sinha†, 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†, N. Govindarajan†, 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

4 **Using pH dependence for understanding mechanisms in electrochemical CO reduction**, *G. Kastlunger, L. Wang, N. Govindarajan, H. H. Heenen, T. F. Jaramillo, C. Hahn, and K. Chan*, In preparation, (2021).

3 **Rationalizing trends in potential of zero charge on transition metal surfaces using Ab-Initio Molecular Dynamics Simulations**, *S. R. Kelly, H. H. Heenen, N. Govindarajan, K. Chan, and J. K. Nørskov*, In preparation, (2021).

2 **Effect of different monomer precursors with identical functionality on the properties of the polymer network**, *A. Torres-Knopp, V. Schamboeck, N. Govindarajan, P. D. Iedema, and I. Kryven*, *Commun Mater*, 2, 50 (2021).

1 **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).

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

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*.

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.*

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, LaTeX, Shellscript, 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