CURRICULUM VITAE

PERSONAL INFORMATION

Name	**Dr. YOGESHWARAN KRISHNAN**
Address	**470 K. Bandarapalli** **Tirupattur** **635854, India** **Phone: +91 9566875921** **https://yogkr.github.io/**
Email	yogeshwara18@gmail.com
Nationality	Indian
Sex	Male

OBEJECTIVE

- Experienced researcher with a Ph.D. and more than 9 years of experience in MM, MD, DFT, AIMD, MLMD applied to complex chemical and material systems. Skilled in computational method development, data analysis, and scientific problem solving, with a strong record of interdisciplinary collaboration and knowledge. Passionate about advancing research in computational chemistry and physics through innovation. My long-term goal is to become a professor, contributing to cutting-edge research and the training of future scientists

ACADEMIC BACKGROUND

• Degree	Postdoctoral Research Associate
• Thesis Title	Machine Learning potentials for solid-liquid interface materials
• Advisor	Assoc. Prof. Heine A Hansen
• University	Technical University Denmark, Denmark
• Degree	Doctor of Philosophy
• Thesis Title	The molecular simulation of energy-transfer processes at interfaces
• Advisor	Prof. Niall J. English
• University	University College Dublin, Ireland
• Degree	Master of Science - Materials Science
• College	PSG College of Technology, Coimbatore
• University	Anna University, Chennai

• Degree	Bachelor of Science - Physics
• College	Sacred Heart College, Tirupattur
• University	Thiruvalluvar University, Vellore

PUBLICATIONS

• Submitted

- CURATOR: Building Robust Machine Learning Potentials for Atomistic Simulations Autonomously with Batch Active Learning
  Xin Yang, Martin Hoffmann Petersen, Renata Sechi, William Sandholt Hansen, Sam Walton Norwood, Yogeshwaran Krishnan, Smobin Vincent, Jonas Busk, Francois Raymond J Cornet, Ole Winther, Juan Maria Garcıa Lastra, Tejs Vegge, Heine Anton Hansen, Arghya Bhowmik **Nat. Mach. Intell.** ***
- Tetrazole functionalization: A new strategy toward stable ion-solvating polymer electrolytes for alkaline water electrolysis
  Dmytro Serhiichuk ,Sinu C. Rajappan, Yogeshwaran Krishnan, Yifan Xia ,Mikkel Rykær Kraglund, Heine Anton Hansen ,Jens Oluf Jensen, David Aili **Adv. Energy Mater.** ***
- A Machine Learning Perspective on the First Step of the Oxygen Reduction Reaction on Au(100)
  Yogeshwaran Krishnan and Heine A Hansen **Adv. Energy Mater.** ***

• Published

- Unifying the Oxygen Reduction and Evolution Reaction with Surface Oxygen and Extracting their Intrinsic Activities on Platinum Catalysts
  Benedikt A Brandes, Yogeshwaran Krishnan, Fabian L Buchauer, Heine A Hansen and Johan Hjelm **Nat. Commun.** 15, 7336 (2024)
- Ultralow Fe instigated defect engineering of hierarchical N–Porous carbon for highly efficient electrocatalysis
  Kiran P Shejale, Yogeshwaran Krishnan, Ranjith Kumar Dharman, Yeon Uk Jeong, Sung Yeol Kim **Mater. Des** 227, 111782 (2023)
- Controlling hydrogen release from remaining-intact Clathrate hydrates by electromagnetic fields: molecular engineering via microsecond non-equilibrium molecular dynamics
  Yogeshwaran Krishnan, Patricia Gomez Rosingana, Mohammad Reza Ghaani and Niall J. English, **RSC Adv.** 12, 4370 (2022)
- Self-Diffusion of Individual Adsorbed Water Molecules at Rutile (110) and Anatase (101) TiO2 Interfaces from Molecular Dynamics
  Stephanie J. Boyd, Dáire OCarroll , Yogeshwaran Krishnan,Run Long, Niall J. English **Crystals** 12(3), 398 (2022)
- Determination of inclusion geometry of cyclodextrin host-guest complexes: Applicability of 1D selective NMR methods
  Deepak Kumar, Yogeshwaran Krishnan, Manikandan Paranjothy, and Samanwita Pal **J. Magn. Reson. Open** 10-11, 100053 (2022)
- Hydrogen and Deuterium Molecular Escape from Clathrate Hydrates:“Leaky” Microsecond-Molecular-Dynamics Predictions
  Yogeshwaran Krishnan, Mohammad Reza Ghaani, Niall J English **J. Phys. Chem. C** 125 (15), 8430 (2021)

- Influence of external static and alternating electric fields on self-diffusion of water from molecular dynamics

  Stephanie J Boyd, Yogeshwaran Krishnan, Mohammad Reza Ghaani, Niall J English **J. Mol. Liq.** 327, 114788 (2021)

- Oxygen-evolution reactions (OER) on transition-metal-doped $Fe_3Co(PO_4)_4$ iron-phosphate surfaces: a first-principles study

  Yogeshwaran Krishnan, Sateesh Bandaru, Niall J English **Catal. Sci. Technol.** 11, 4619 (2021)

- Vibrational Spectra of a N719-Chromophore/Titania Interface from Empirical-Potential Molecular-Dynamics Simulation, Solvated by a Room Temperature Ionic Liquid

  Yogeshwaran Krishnan, Aaron Byrne and Niall J. English, **J. Vis. Exp** 155, e60539 (2020)

- Electric-Field Control of Neon Uptake and Release to and from Clathrate Hydrates

  Yogeshwaran Krishnan, Mohammad Reza Ghaani and Niall J. English, **J. Phys. Chem. C** 123, 27554 (2019)

- Ab Initio Molecular Dynamics Studies of the Effect of Solvation by Room-Temperature Ionic Liquids on the Vibrational Properties of a N719-Chromophore/Titania Interface

  Aaron Byrne, Yogeshwaran Krishnan and Niall J. English, **J. Phys. Chem. A** 122, 26464 (2018)

- Vibrational Study of Iodide-Based Room-Temperature Ionic-Liquid Effects on Candidate N719-Chromophore/Titania Interfaces for Dye-Sensitised Solar-Cell Applications from Ab-Initio Based Molecular-Dynamics Simulation

  Yogeshwaran Krishnan, Aaron Byrne and Niall J. English, **Energies** 11(10), 2570 (2018)

- Theoretical study of perbenzoate anion decomposition pathways in the gas phase

  Yogeshwaran Krishnan, Pranay Rajbangshi and Manikandan Paranjothy, **Int. J. Mass Spectrom.** 428, 8 (2018)

- Classical dynamics simulations of interstellar glycine formation via CH_2 = NH + CO + H_2O reaction

  Yogeshwaran Krishnan, Allen Vincent and Manikandan Paranjothy, **J. Chem. Sci.** 129, 1571 (2017)

- Classical Dynamics Simulations of Dissociation of Protonated Tryptophan in the Gas Phase

  Yogeshwaran Krishnan, Nishant Sharma, Upakarasamy Lourderaj and Manikandan Paranjothy, **J. Phys. Chem. A** 123, 4389 (2017)

- Analysis of Molecular Interaction of Drugs within β -Cyclodextrin Cavity by Solution-State NMR Relaxation

  Deepak Kumar, Yogeshwaran Krishnan, Manikandan Paranjothy, and Samanwita Pal **J. Phys. Chem. B** 121, 2864 (2017)

RESEARCH/TEACHING EXPERIENCE

Teaching Assistant

• Subject	Introduction to Engineering Computing (MATLAB)
• University	University College Dublin, Dublin, Ireland

Research Fellow

• Research Title	Chemical dynamics simulations of complex organic reactions: Mechanistic insights and microsolvation effects
• Advisor	Dr. Manikandan Paranjothy
• University	Indian Institute of Technology Jodhpur, Jodhpur, India
•	Computational Science

RESEARCH INTERESTS

- Machine Learning
- Molecular Dynamics
- Electronic Structure Theory
- Chemical Reaction Dynamics
- Computational Material Science

FUNDING

- Non-equilibrium Dynamics at the Solid-Liquid Interface accelerated by Neural Network Potentials (PI), GPU-CPU hours worth 1.3 M, Large Unified Modern Infrastructure (LUMI) Finland.

CONFERENCES/WORKSHOPS

- Participated in workshop on **The Catalysis and Modeling Symposium** September 12-14, 2022, DK
- Participated in workshop on **DL_Software Training** December 4-6, 2019, Molecular Sciences Research Hub (MSRH) University College London, London, UK
- Participated in workshop on **VASP Workshop: Electronic Structure Modelling for Surface and Interface Science** October 22-23, 2019, Riverside Innovation Centre, University of Chester, Chester, UK

COMPUTATIONAL SKILLS

• Operating Systems	Linux, Windows, MacOS
• Programming Languages	Python, Shell scripting, LaTeX
• Software	AMBER, DL_POLY, GROMACS, GAMESS, Gaussian, NWChem, VASP

REFERENCES

• Name	Heine A. Hansen
• Position	Associate Professor
• Electronic Address	heih@dtu.dk
• Mailing Address	Department of Energy Conversion and Storage Technical University of Denmark 2800 - Denmark.
• Name	Manikandan Paranjothy
• Position	Professor
• Telephone	+91-291-2801306
• Electronic Address	pmanikandan@iitj.ac.in
• Mailing Address	Department of Chemistry Indian Institute of Technology Jodhpur Jodhpur 342037 - India.
• Name	Ananya Debnath
• Position	Professor
• Telephone	+91-291-2801307
• Electronic Address	ananya@iitj.ac.in
• Mailing Address	Department of Chemistry Indian Institute of Technology Jodhpur Jodhpur 342037 - India.
• Name	Niall J. English
• Position	Professor
• Telephone	+353-17161646
• Electronic Address	niall.english@ucd.ie
• Mailing Address	School of Chemical and Bio-process Engineering University College Dublin Belfield, Dublin 4 - Ireland