CURRICULUM VITAE

PERSONAL INFORMATION

Name	**Dr. YOGESHWARAN KRISHNAN**
Address	**Postdoctoral Researcher** **Department of Energy Conversion and Storage** **Technical University of Denmark** **Lyngby, 2800, Denmark** **https://yogkr.github.io/**
Email	yogeshwaran.krishna@gmail.com
Nationality	Indian
Sex	Male

ACADEMIC BACKGROUND

• Degree	Postdoctoral Research Associate
• Year	2024
• 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
• Year	2021
• 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
• Year	2014
• College	PSG College of Technology, Coimbatore
• University	Anna University, Chennai
• Degree	Bachelor of Science - Physics
• Year	2012
• College	Sacred Heart College, Tirupattur
• University	Thiruvalluvar University, Vellore

PUBLICATIONS

• Published

- 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)
- 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)
- 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)
- 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)
- 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)
- 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)
- 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)
- 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)
- 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)
- 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)
- 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)

- 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)
- 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)
- 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)
- 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 **Elsevier Materials and Design** 227, 111782 (2023)

• Submitted

- 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.** *** (2023)
- 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.** *** (2024)
- etrazole 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.** *** (2024)
- 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.** *** (2024)

RESEARCH/TEACHING EXPERIENCE

Teaching Assistant

- Date: Sep. 2018 - Jan. 2020
- Subject: Introduction to Engineering Computing (MATLAB)
- University: University College Dublin, Dublin, Ireland

Research Fellow

- Date: Jan. 2018 - Apr. 2018
- Research Title: Bandgap engineering and surface studies of semiconductors for gas sensing applications
- Advisor: Dr. Mahesh Kumar

• University	Indian Institute of Technology Jodhpur, Jodhpur, India
	Research Fellow
• Date	Oct. 2014 - Jan. 2018
• 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

FIELD OF SPECIALIZATION

- Computational Science

RESEARCH INTERESTS

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

CONFERENCES/WORKSHOPS

- 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
- Poster presentation entitled Gas Phase Classical Dynamics Simulations of Protonated Tryptophan, **North West meeting on Spectroscopy, Structure and Dynamics 2017**, March 18-19, 2017, BITS Pillani, Rajasthan, India
- Poster presentation entitled Post Annealing Effect of Tellurium Rich Bi_2Te_3 Thin Film By E-Beam Evaporation Technique
  National conference on functional materials (NCFM) May 23-24, 2014, PSG College of Technology Coimbatore, Tamil Nadu, India
- Participated in workshop on **Non Linear Dynamics**
  December 1-21, 2016, PSG College of Technology Coimbatore,Tamil Nadu, India
- Participated in workshop on **Emerging Trends in Materials science, Nanoscience and Nanotechnology**
  PSG College of Technology Coimbatore,Tamil Nadu, India

COMPUTATIONAL SKILLS

• Operating Systems	Linux, Windows, MacOS
• Programming Languages	Python, Shell scripting, LaTeX
• Software	DL_POLY, GROMACS, VENUS, 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	Juan Maria García Lastra
• Position	Professor, Head of section
• Electronic Address	jmgla@dtu.dk
• Mailing Address	Department of Energy Conversion and Storage Technical University of Denmark 2800 - Denmark.
• 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
• 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.