Akhil S. Nair

+49-1553432518 e-mail linkedin twitter gitlab orcid website

PERSONAL PROFILE

Date of Birth: May 13, 1994
Gender: Male
Address: Grunstrasse 7, Kopenick, 12555 Berlin
Nationality: Indian
Marital Status: Single
Languages: English, Hindi, Malayalam, Tamil, German

RESEARCH EXPERIENCE

Postdoctoral Researcher **August 2022 – Present**
Supervision: Prof. Matthias Scheffler *NOMAD Lab, Fritz-Haber Institute of the Max-Planck Society*
Research Area: AI-driven material discovery

Research Associate **May 2022 – July 2022**
Research Guide: Prof. Biswarup Pathak *Computational Materials Designing Group,IIT Indore*
Research Area: Computational catalysis

Ph.D. Thesis Work **May 2017 – March 2022**
Thesis Supervisor: Prof. Biswarup Pathak *Computational Materials Designing Group,IIT Indore*
Thesis title: Developing computational strategies for platinum nanocatalyst based fuel cell applications

Visiting Research Fellow **August 2022 – November 2022**
Supervision: Prof. Rajeev Ahuja *Department of Physics and Astronomy, Uppsala University, Sweden*
Research Area: Energy materials

Master's Thesis Work **January 2016 – August 2016**
Thesis supervisor: Prof. E. G. Jayasree *Department of Chemistry, University of Kerala*
Thesis title: DFT study of Lithium Enethiolate Aggregates

Summer Research Fellow **May 2015 – July 2015**
Project supervisor: Prof. E. Arunan *IPC Department, Indian Institute of Science, Banglore*
Project topic: Theoretical study of intermolecular complexes of third period elements

EDUCATION

Ph.D. Computational Chemistry **May 2017 – March 2022**
Grade: 8.28/10 *Department of Chemistry, IIT Indore, India*

Master of Science, Chemistry **July 2014 – August 2016**
Grade: 7.5/10 *Department of Chemistry, University of Kerala, India*

Bachelor of Science, Chemistry **July 2011 – June 2014**
Grade: 3.5/4 *Mar Ivanios College, University of Kerala, India*

HONORS/AWARDS

- August 2022 - Decembet 2023: Max-Planck postdoctoral fellowship from Fritz-Haber Institute of the Max-Planck Society, Berlin Germany
- 2019, 2022 : Visiting research fellowship from Department of Physics and Astronomy, Uppsala University, Sweden
- 2017: Qualified the National Level Exam, Graduate Aptitude Test in Engineering (GATE), India
- 2017: Selected for Orientation Course for Engineering Graduates and Science Postgraduates (OCES) program at Bhabha Atomic Research Center, India
- 2017: Awarded Kerala State Council for Science, Technology and Environment (KSCSTE) Research Fellowship
- 2016: Qualified the National Level Exam, CSIR-NET fellowship, India

CONFERENCES/WORKSHOPS/HACKATHONS

- DPG Meeting of the Condensed Matter Section in Dresden, Germany, March, 17-22, 2024
  Talk: *Leveraging Multi-Fidelity Data In AI-Driven Sequential Learning of Materials Properties: Identifying Stable Water Splitting Catalysts*
- Acceleration Consortium Bayesian Optimization Hackathon, March, 27-28, 2024
  Project: *Investigation of Multi-Objective Bayesian Optimization of QM9 Dataset*
- CECAM/Psi-k conference on *Bridging length scales with machine learning: from wavefunctions to thermodynamics*, Freie University of Berlin, June, 19-23, 2023
- School on Artificial Intelligence for Materials Science in the Exascale Era, May 21 - 26, 2023
  Poster: *Non-Local DFT calculations towards the discovery of stable water-splitting catalysts*
- ASE Hackathon: *Generalising and improving simulation code interfaces*, Technical University of Denmark, March, 20-24, 2023
- DPG Meeting of the Condensed Matter Section in Dresden, Germany, March, 26-31, 2023
  Talk: *Non-Local DFT calculations towards the discovery of stable water-splitting catalysts*
- University of Kerala, India, March 19, 2022
  Talk: *Computational designing of materials for energy applications*
- Government PG College Berinag, India, August 14-16, 2021
  Talk: *Computational designing of molecules and materials*
- Theoretical Chemistry Symposium 2021, IISER Kolkata, India, December 11-14, 2021
  Poster: *Refining theoretical frameworks for nanocluster catalysis*
- Workshop on *Accelerated Machine Learning and Deep Learning with Intel*, Berlin, March 8-9, 2023
- IKZ-FAIRmat winter school on *Machine learning in materials science and crystal growth*, Berlin, January 23-25, 2023.
- Workshop and Symposium on *Advanced Simulation Methods: DFT, MD and Beyond*, IIT Delhi, India, March 6-10, 2019
- Mumbai Workshop on *Quantum Chemistry and Density functional theory*, IIT Bombay, India, June 5-9, 2019
- Asia-Pacific Conference of Theoretical and Computational Chemistry 2017,IIT Bombay, India, December 15-17, 2017
  Poster: *Multilayered Platinum Nanotube for Oxygen Reduction in a Fuel Cell Cathode*

PUBLICATIONS

1. Gratious, S., Afreen, Mahal, E., Thomas, J., Saha, S., **Nair, A.S.**, Adarsh, K. V., Pathak, C.*, Mandal, S.* (2024): "Visualizing" the partially reversible conversion of gold nanoclusters via the Au23(S-c-C6H11)17 intermediate. Chem. Sci., 2024.

2. Mondal, B., Jana, A., Roy, J., Mata, A. C., **Nair, A.S.**, Mahendranath, A., Roy, S., Pathak, B., Ajayan, P.M., Pradeep, T. (2023): ACS Materials Lett., 5, 12, 3306–3315

3. Jose, A., Jana, A., Gupte, T., **Nair, A.S.**, Unni, K., Nagar, A., Kini, A. R., Spoorthi, B.K., Jana, S.K., Pathak, B.*, Pradeep, T.* (2023): Vertically Aligned Nanoplates of Atomically Precise Co6S8 Cluster for Practical Arsenic Sensing. ACS Materials Lett., 5, 3, 893–899.

4. Mukherjee, S., Das, A., Das, A.K., Sheriff, A., Sunny, K., **Nair, A.S.**, Bhandary, S., Bhowal, R., Chopra, D., Pathak, B., Yamazoe, S., Mandal, S.* (2023): Single Cu Atom Doping on Au11 Nanocluster: Its Implication toward Selectivity in C–C Coupling Reaction. Chem. Mater., 35, 4, 1659–1666.

5. Sharma, R.K., **Nair, A.S.**, Bharadwaj, N., Roy, D., Pathak, B.* (2023): Role of Fluxionality and Metastable Isomers in the ORR Activity: A Case Study. J. Phys. Chem. C, 127, 1, 217–222.

6. Jana, A., Spoorthi, B.K., **Nair, A.S.**, Nagar, A., Pathak, B., Base, T., Pradeep, T. (2023): A Luminescent Cu4 Cluster Film Grown by Electrospray Deposition: A Nitroaromatic Vapour Sensor, Nanoscale. Accepted Manuscript.

7. Mandal, S.C., Das, A., Roy, D., Das, S., **Nair, A.S.**, Pathak, B.* (2022): Developments of the heterogeneous and homogeneous CO2 hydrogenation to value-added C2+-based hydrocarbons and oxygenated products. Coord. Chem. Rev., 471, 214737.

8. **Nair, A.S.**, Pathak, B.* (2022): Accounting for Dispersion Effects in DFT Framework of Electrocatalysis: A Case Study of Solvent Mediated Oxygen Reduction Reaction. J. Phys. Chem. C, 126, 6171–6188.

9. Bharadwaj,N. **Nair, A.S.**, Das, S., Pathak, B.* (2022): Size-Dependent Effects in Fullerene-Based Catalysts for Nonaqueous Li–Air Battery Applications. ACS Appl. Energy Mater., 5, 3, 3380–3391.

10. **Nair, A.S.**, Anoop, A., Ahuja, R., Pathak, B.* (2022) Relativistic effects in platinum cluster catalysis: A statistical ensemble-based approach. J. Phys. Chem. A, 126, 1345–1359.

11. Das, A. K., Biswas, S., Wani, V. S., **Nair, A.S.**, Pathak, B., Mandal, S.* (2022): [Cu18H3(S-Adm)12(PPh3)4Cl2]: fusion of Platonic and Johnson solids through a Cu(0) center and its photophysical properties, Chem. Sci., 13, 7616.

12. Das, A. K., Mekkat, R., Maity, S., **Nair, A.S.**, Bhandary, S., Bhowal, R., Patra, A., Pathak, B., Chopra, D., Mandal, S* (2021): Role of Ligand on Photophysical Properties of Nanoclusters with fcc Kernel, Inorg. Chem., 60, 24, 19270–19277.

13. Das, A., Mandal, S. C., **Nair, A.S.**, Pathak, B* (2022): Computational Screening of First-Row Transition-Metal Based Alloy CatalystsLigand Induced N2 Reduction Reaction Selectivity. ACS Phys. Chem Au, 2, 2, 125–135.

14. Gratious, G., **Nair, A.S.**, Mukherjee, S., Kachappilly, N., Pathak, B., Mandal, S*. (2021): Gold Deassembly: From Au44(SPh-tBu)28 to Au36(SPh-tBu)24 Nanocluster through Dynamic Surface Structure Reconstruction. J. Phys. Chem. Lett., 12, 45, 10987–10993.

15. Bharadwaj, N., **Nair, A.S.** Pathak, B*. (2021): Dimensional-Dependent Effects in Platinum Core–Shell-Based Catalysts for Fuel Cell Applications. ACS Appl. Nano Mater. 4, 9, 9697–9708.

16. **Nair, A.S**., Pathak, B.* (2021): Computational strategies to address the catalytic activity of nanoclusters. Wiley Interdiscip. Rev. Comput. Mol. Sci., 11, e1508.

17. Das, A., **Nair, A. S.**, Mandal,S. C., Pathak, B* (2021): Current Density Calculations of an Octahedral Fe Nanocluster for Selective Electrocatalytic for Nitrogen Reduction. ACS Appl. Nano Mater. 4, 8, 7758–7770

18. Das, A. K., Biswas, S., Thomas, A., Paul, S., **Nair, A. S.**, Pathak, B., Singh, M. S., Mandal, S.* (2021): Switchable photon and phonon emission properties of an atomically precise Ag14 core-based two-dimensional silver cluster-assembled material. Mater. Chem. Front., 5, 8380-8386.

19. **Nair, A.S**., Anoop, A., Ahuja, R., Pathak, B.* (2021): Role of atomicity in the oxygen reduction reaction activity of platinum sub nanometer clusters: A global optimization study. J. Comp. Chem., 4, 084201

20. Nandi, S., **Nair, A.S.**, Pathak, B. (2020): First principles investigation on the applicability of ruthenium as a potential ORR catalyst. J Chem. Sci., 132, 2.

21. Das, A. K., Mukherjee, S., R, S. S., **Nair, A. S.**, Bhandary, S., Chopra, D., Sanyal, D., Pathak, B., Mandal, S.* (2020): Defects Engineering on Ceria and C–C Coupling Reactions Using [Au11(PPh3)7I3] Nanocluster: A Combined Experimental and Theoretical Study. ACS Nano, 14, 16681–16688

22. Maman, M. P., **Nair, A.S**., Nazeeja, A. M. A. H., Pathak, B., Mandal, S.* (2020): Synergistic Effect of Bridging Thiolate and Hub Atoms for the Aromaticity Driven Symmetry Breaking in Atomically Precise Gold Nanocluster. J. Phys. Chem. Lett., 11, 10052–10059.

23. Maman, M. P., **Nair, A. S.**, Cheraparambil, H., Pathak, B.*, Mandal, S.* (2020): Size Evolution Dynamics of Gold Nanoclusters at an Atom-Precision Level Ligand Exchange, Growth Mechanism, Electrochemical and Photophysical Properties. J. Phys. Chem. Lett., 11, 5, 1781-1788.

24. Das, A., **Nair, A. S.**, Pathak, B.* (2020): Elucidating Mechanistic Origin of the Catalytic Activity of the Fe(111) Surface and Nanoclusters toward the Electrochemical Nitrogen Reduction Reaction. J. Phys. Chem. C, 124, 37, 20193-20202

25. **Nair, A. S.**, Ahuja, R.,Pathak, B.* (2020): Unraveling the single-atom electrocatalytic activity of transition metal-doped phosphorene. Nanoscale Adv., 2, 8, 2410-2417

26. Garg, P., **Nair, A. S.**, Rawat, K. S., Pathak, B.* (2019): Computational Screening of Electrocatalytic Activity of Transition Metal-Doped CdS Nanotubes for Water Splitting. J. Phys. Chem. C, 123, 22, 13419-13427

27. **Nair, A. S.**, Pathak, B.* (2019): Computational Screening for ORR Activity of 3d Transition Metal Based M@Pt Core–Shell Clusters. J. Phys. Chem. C, 123, 6, 3634-3644

28. Mahata, A., **Nair, A. S.**, Pathak, B.* (2019): Recent advancements in Pt-nanostructure-based electrocatalysts for the oxygen reduction reaction. Catal. Sci. Technol., 9, 17, 4835-4863

29. George, A., Sundar, A., **Nair, A. S.**, Maman, M. P., Pathak, B., Ramanan, N., Mandal, S.* (2019): Identification of Intermediate Au22(SR)4(SR)14 Cluster on Ligand-Induced Transformation of Au25(SR)18 Nanocluster. J. Phys. Chem. Lett. 10, 16, 4571-4576

30. **Nair, A.S**., Mahata, A, Pathak, B.* (2018): Multilayered platinum nan- otube for oxygen reduction in a fuel cell cathode: Origin of activity and product selectivity, ACS Appl. Ener. Mat., 1, 8, 3890–3899.

TEACHING

Teaching Assistant at Indian Institute of Technology Indore

Postgraduate course : Quantum Chemistry and Group theory

Undergraduate course : Thermodynamics

SKILLS & EXPERTISE

Electronic structure codes: FHI-aims, GPAW, VASP, Quantum Espresso, Gaussian, ORCA, SIESTA, XTB

Machine learning tools: Sklearn, PyTorch, TensorFlow, BoTorch, SISSO, Subgroup Discovery

Computational expertise: parallel computing, high-performance computing, Git, Gitlab

Programming: Python, R, Bash scripting, HTML

Operating systems: Linux, Windows

Text editors: Vim, Nano, Atom, Visual Studio Code, Emacs

Text formatting: Latex, Markdown, MS Word, LibreOffice Writer

REFERENCES

Prof. Matthias Scheffler
Professor & Director
Novel Materials Discovery (NOMAD) Lab
Fritz-Haber Institute of the Max-Planck Society
Faradayweg 4-6, 14195 Berlin
Contact: +49 30 8413 4711
Email: scheffler@fhi-berlin.mpg.de

Dr. Anoop Ayyappan
Associate Professor
Department of Chemistry
Indian Institute of Technology, Kharagpur
West Bengal-721301
Contact: +91 (22) 9383414629
Email: anoop@chem.iitkgp.ac.in

Prof. Biswarup Pathak
Professor & Head
Department of Chemistry
Indian Institute of Technology Indore, Simrol
Indore-453552
Contact: +91 0731 2438 772
Email: biswarup@iiti.ac.in

Dr. Sukhendu Mandal
Associate Professor
Department of Chemistry
IISER Trivandrum, Trivandrum
Kerala-695561
Contact: +91 (0)471-2778107
Email: sukhendu@iisertvm.ac.in