KARTHIKRAJA E

Postdoctoral Fellow
Institute for Chemical Reaction Design and Discovery (ICReDD)
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EDUCATION

Ph.D.	Computational Chemistry	AcSIR, CSIR-CLRI Campus	2021-2025
M.Sc.	Chemistry	Pondicherry University	2012-2014
B.Sc.	Chemistry	Bharathiar University	2009-2012

RESEARCH EXPERIENCE

1. **Postdoctoral Fellow (Jun 2025 – Present)**
   Under the mentorship of **Prof. Tetsuya Taketsugu,** ICReDD, Hokkaido University, Sapporo, Japan.
   Project: Mitsui Chemicals
   (1) Development of analysis techniques for surface reactions with solid catalysts
   (2) Computational chemistry research on chemical recycling of polyolefins

2. **Ph.D. Research Scholar (Jan 2021 – May 2025)**
   Under the guidance of **Prof. V. Subramanian,** *Visiting Faculty, Department of Chemistry, IIT Madras, Former Outstanding Scientist, CSIR-CLRI* and **Dr. V.G. Vaidyanathan**, *Principal Scientist, CSIR-CLRI*.
   Thesis title: *"Computational Studies on Design and Development of Novel Two-Dimensional Materials for Energy Storage and Conversion Applications"*

3. **Project Assistant II (Jan 2018 – Mar 2020)**
   Under the guidance of **Dr. T Raja,** Principal Scientist, at the Catalysis and Inorganic Chemistry division, CSIR-NCL, Pune.
   Project title: *"CSIR-Mission Mode (MM) Project- Catalysis for Sustainable Development (CSD)"*

4. **Master's Research Project (2014)**
   Under the guidance of **Prof. Tharanikkarasu Kannan,** *Department of Chemistry, Pondicherry University, Puducherry.*
   Project title: *"Synthesis of Novel Isoniazid Derivatives as Anti-tuberculosis Agents"*

RESEARCH FOCUS

- **Batteries:** Design of 2D Dirac materials as anode materials for lithium-ion batteries.
- **Thermoelectric Application:** Design of novel 2D carbon allotropes for thermoelectric applications.
- **Electrocatalysis:** Design of electrocatalysts for electrochemical Hydrogen Evolution Reaction (HER) and electrochemical Nitrogen Reduction Reaction (NRR).

TECHNICAL SKILLS

- VASP: Vienna Ab initio Simulation Package
- Quantum ESPRESSO: opEn-Source Package for Research in Electronic Structure, Simulation, and Optimization
- Gaussian 16
- Materials Studio, VTST, LOBSTER, VESTA, GaussView, OriginLab,
- Basic knowledge of Python programming and Machine Learning

PUBLICATIONS

Google Scholar: Number of publications: 08 Number of citations: 31 h-index: 03

1. **Karthikraja, E.**, Nulakani, N. V. R.; Devi, P.; Murugan, P.; Kothandaraman R.; Vaidyanathan, V. G.; Subramanian, V. First-principles insights into biphenylene-based graphynes: promising novel two-dimensional carbon allotropes for thermoelectric applications. *J. Chem. Sci.* **2025** 137, 29. https://link.springer.com/article/10.1007/s12039-025-02361-2
2. G, N. B.; Lazuli, A. R. S. C.; Ramalingam, V.; **Karthikraja, E.**; Poonchi Sivasankaran, R.; Choi, W.; Neppolian, B. Egg Shell Mediated Ni_5P_4/Polypyrrole Electrocatalyst for Sustainable Water Splitting. *Energy & Fuels* **2025**, 39 (1), 750–763. https://doi.org/10.1021/acs.energyfuels.4c03688
3. **Karthikraja, E.**; Chowdhury, C.; Nulakani, N. V. R.; Ramanujam, K.; Vaidyanathan, V. G.; Subramanian, V. Transition Metal Anchored Novel Holey Boron Nitride Analogues as Single-Atom Catalysts for the Hydrogen Evolution Reaction. *Chem Asian J* **2024**, e202401256. https://doi.org/10.1002/asia.202401256
4. Chowdhury, C.; **Karthikraja, E.**; Subramanian, V. DFT and Machine Learning Guided Investigation into the Design of New Dual-Atom Catalysts Based on α-2 Graphyne. *Phys. Chem. Chem. Phys.* **2024**, *26* (38), 25143–25155. https://doi.org/10.1039/D4CP03171G
5. **Karthikraja, E.**; Nulakani, N. V. R.; Choutipalli, V. S. K.; Chowdhury, C.; Murugan, P.; Vaidyanathan, V. G.; Subramanian, V. Acetylene-Mediated Borophosphene Dirac Materials as Efficient Anode Materials for Lithium-Ion Batteries. *ChemPhysChem* **2023**, *24* (11), e202300035. https://doi.org/10.1002/cphc.202300035
6. Choutipalli, V. S. K.; **Karthikraja, E.**; Varathan, E.; Subramanian, V. Vacancy Defect Assisted Enhanced Nitrogen Fixation in Boron Nitride Nanomaterials. *Appl Surf Sci* **2022**, *602*, 154406. https://doi.org/10.1016/j.apsusc.2022.154406
7. Choutipalli, V. S. K.; **Karthikraja, E.**; Subramanian, V. Nitrogen Fixation at the Edges of Boron Nitride Nanomaterials: Synergy of Doping. *Front Chem* **2022**, *9,* 799903. https://doi.org/10.3389/fchem.2021.799903
8. Gupta, N. N.; Punekar, A. S.; **Karthikraja, E.**; Ghodekar, M. M.; Patil, V. S.; Gopinath, C. S.; Raja, T. Phase Transfer Ceria-Supported Nanocatalyst for Nitrile Hydration Reaction. *ACS Omega* **2019**, *4* (14), 16037–16044. https://doi.org/10.1021/acsomega.9b02173

ACHIEVEMENTS

- Qualified the GATE (Chemistry) at all India Level in 2020.

CONFERENCES

- International school and conference on Evolution of Electronic Structure Theory and Experimental Realization (**EESTER-2025, 4th Edition**) jointly organized by SRM Institute of Science & Technology and IIT Madras, Chennai, India, held from January 3 - 11, 2025.
- Theoretical Chemistry Symposium (**TCS-2023**) organized by IIT Madras Chennai, India, held between 07-10 December 2023.
- International Conference on Systems and Processes in Physics, Chemistry and Biology (**ICSPPCB-2023**) organized by Assam University, Silchar, India, held between 02-04 March 2023.
- Theoretical Chemistry Symposium (**TCS-2021**) organized by IISER Kolkata, IACS Kolkata, Kalyani University and S.N. Bose National Centre for Basic Sciences Kolkata held between 11 - 14 December 2021.

REFERENCES

1. **Prof. V. Subramanian, FASc, FNASc,**
   Visiting Faculty,
   Department of Chemistry, IIT Madras,
   Former Outstanding Scientist,
   CSIR-Central Leather Research Institute,
   Chennai - 600 036, Tamil Nadu, India,
   Email: subramanianv@iitm.ac.in
   subuchem@hotmail.com

2. **Dr. V.G. Vaidyanathan**
   Principal Scientist,
   Advanced Materials Laboratory,
   CSIR-Central Leather Research Institute,
   Chennai - 600 020, Tamil Nadu, India,
   Email: vaidyanathan@clri.res.in

3. **Prof. Tetsuya Taketsugu**
   Quantum Chemistry Laboratory,
   Department of Chemistry,
   Faculty of Science, Hokkaido University,
   Institute for Chemical Reaction Design
   and Discovery (WPI-ICReDD),
   Hokkaido University, N10-W8, Kita-ku,
   Sapporo 060-0810, Japan
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