Indian | Ph: +91●759●846●4724 | e-mail: maheraj435878@gmail.com, dmahendiran@cecri.res.in

D. Mahendiran

Central Electrochemical Research Institute (CSIR Laboratory), India

Education

Ph.D. (Physical Sciences), Pursuing

- CSIR-CECRI, India

Master of Science (Physics), 2016

- The Gandhigram Rural Institute (Deemed University), India

Awards

- **UGC NET JRF** June 2018 – Award no : 1393/(CSIR-UGC NET June 2018)
- State Eligibility Test for Assistant Professor (SET 2018).

Software Proficiency

- **Computation**

  Parallel Programming: OpenMP, MPI
  System Administration: Handling of Linux Clusters and Software Installations.
  Programming Language: Python, Shell script.
- **Software** : VASP, Quantum ESPRESSO, Wien2K, Phonopy, wannier90, Materials Studio. Materials Project Database.
- **Writing**: Latex, Mendeley, EndNote.

Supervisors References

Dr. P. Murugan
Principal Scientist,
CSIR-Central Electrochemical Research Institute, India.
e-mail: murugan@cecri.res.in
palanichamymurugan@gmail.com

Dr. M. Sathish,
Senior Scientist,
CSIR-Central Electrochemical Research Institute, India.
e-mail: msathish@cecri.res.in
marappan.sathish@gmail.com

Interest

Computational Investigaions on

- Energy Materials (Batteries), Energy Conversion and Catalysis.
- Screening the Materials using High-Throughput Computing Method (Data Screening for Existing Database).
- Low Dimensional Nanostructures (Nanotubes and Nanoribbon).
- vdW Heterostructures and Properties.

Research Experiences

- Density functional theory calculations for exfoliation of layers from covalently bonded bulk system and assessing optoelectronic properties.
- Effcient energy storage materials screening from database..

Published papers

1. The Role of Defects Presenting in Graphitic SiC Sheets and their Consequences in the Exfoliation of Layers – A First Principles Approach (*Phys. Chem. Chem. Phys., 2022*)
2. Highly Conductive $NiSe_2$ Nanoparticle as a Co-catalyst Over TiO_2 for Enhanced Photocatalytic Hydrogen Production (*Applied Catalysis B: Environmental.*, 2022, **307**, 121159)
3. High-throughput Computational Screening of Anode Materials for Fluoride ion Batteries using DFT (under peer review, Chem. Mater.)

International Conferences

- International Conference on Evolution of Electronic Structure Theory and Experimental Realization (EESTER -2020) Jointly organized by SRMIST KTR (India), IIT Madras (India) and Uppsala University (Sweden) December 14 – 18 , 2020 in webinar mode.
- 2nd International Conference on Advances in Materials Science (AIMS-2021) organized by Department of Physics (Division of Science and Technology) 05-06 October 2021.

Addtional Courses

- Computational Methods in Physics using Python CoMP-Py 2021 organized by IIT, Allahabad (May - July 2021).
- HPC Shiksha -Basics of High Performance Computing orgnized by NSM Nodal Centres (Nov 2020 – Jan 2021).