Karthikeyan Jeyakumar

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OBJECTIVE

To become an excellent academic researcher in computational materials science that provides opportunities to explore the newer dimensions of low-dimensional materials by adding my creativity and knowledge.

ACADEMIC AND RESEARCH PROFILE

Year	Position	College/Department	Institution/University
Aug2022-	Assistant Professor	Department of Physics	NIT, Durgapur
2020-July2022	DST Inspire Faculty	Department of Sciences and Humanities	RGIPT, Jais, India
2018-2020	Post Doctoral Fellow	Department of Applied Physics	Aalto University, Finland.
2013 – 2018	Research Scholar	Functional Materials Division	AcSIR at CECRI, India
2011 – 2013	Junior Research Fellow	Functional Materials Division	CSIR-CECRI, India
2009 – 2011	PG – Student	School of physics	MK University, India
2006 – 2009	UG – Student	VHNSN College	MK University, India

Thesis Title: "First Principles Calculations on Structural Stability and Physicochemical Properties of Mo-S Nanostructures"
Research Supervisor: **Dr. P. Murugan**, Senior Scientist, CSIR-CECRI, India. **Contact at:** murugan@cecri.res.in

Research Interests

I am strongly motivated to study nanomaterials' physicochemical properties, which can be engineered based on our requirements. First Principles DFT calculations are a powerful tool to deduce the properties of materials. In Dr. P. Murugan's research group, functioning at CSIR-CECRI, I studied 0D, 1D, and 2D structures of Mo-S compounds, to understand their electronic, magnetic, and catalytic properties. In particular, the role of concealed defects is computationally identified in the MoS_2 single layer to explain the better catalytic performance of MoS_2 nanospheres. Also, I understood the role of valance electron concentration (VEC) in Mo-S 1D structures derived from Mo-S atomic clusters. Now I am trying to extend the concept of VEC to other metal sulfide nanowires, which is my dream project. In addition to Mo-S-based materials, I have also worked on some Phosphor materials and Li-ion battery anode materials. With the above experience, I completed my Ph.D. and moved to the applied physics department at Aalto University, Finland. At Aalto, I intensely studied the properties of modified layered materials using density functional theory calculations.

- Growth of 1D and 2D Nanostructures from Atomic Clusters.
- Electronic and Magnetic Structure of Cluster, Nanowires, and Nanosheets.
- Electrochemical Properties of Nanomaterials for energy storage and energy conversion applications.

Teaching and Research Guidance

At NIT Durgapur, I teach Engineering Physics (1 and 2nd Sem) and Physics of Engineering Materials (3rd Sem) to undergraduate students and Condensed Matter Physics II & III, Physics of Nanomaterials, and Photonics to postgraduate students.
I taught Classical Physics (2 Sem) and Modern Physics (1 Sem) to undergraduate students at RGIPT, Jais, India.
I have guided two undergraduate projects at RGIPT, Jais.

Publications [T.C = Total citations = 434(Last 3 years: 268), h-index = 10, i-10 index = 10]

[1] Anwesh Kumar, Hannu-Pekka Komsa, Diksha Praveen Pathak, Balathanigaimani Marriyappan Sivagnanam, ASK Sinha, J Karthikeyan, Origin of Enhanced Photocatalytic Activity in Direct Band Gap g-C_3N_4 Nanoribbons with Tunable Electronic Properties for Water-Splitting Reaction: A First-Principles Study, The Journal of Physical Chemistry C, 126, 46, 19627–19636, (2022).

[2] Logu Thirumalaisamy, Soundarrajan Palanivel, Karthikeyan Jeyakumar, Sethuraman Kunjithapatham, Trystan Watson, Sudhagar Pitchaimuthu, The upsurge of absorption coefficient in $CuInS_2$ thin film with Ru doping: an energetic absorber layer in a superstrate solar cell, Materials Today Chemistry, 26, 101217, (2022).

[3] Saifi, Shadab; Dey, Gargi; Karthikeyan, Jeyakumar; sinha, ASK; Aijaz, Arshad, MoS_2 and WS_2 Nanosheets Decorated on Metal-Organic Framework-Derived Cobalt/Carbon Nanostructures as Electrocatalysts for Hydrogen Evolution, ACS Applied Nano Materials, 5, 8, 10696-10703, (2022).

[4] S Suba Viveka, T Logu, N Ahsan, J. Karthikeyan, P Murugan, M Sampath, S Kalainathan, Arunava Gupta, Y Okada, K Sethuraman, Fe-doped $CuGaS_2$($CuGa_{1-x}Fe_xS_2$)-Detailed analysis of the intermediate band optical response of chalcopyrite thin films based on first principle calculations and experimental studies, Materials Science in Semiconductor Processing, 136, 106133, (2021).

[5] Markus Aapro, Md. Nurul Huda, J. Karthikeyan, Shawulienu Kezilebieke, Somesh C. Ganguli, Héctor González Herrero, Xin Huang, Peter Liljeroth, and Hannu-Pekka Komsa, Synthesis, and Properties of Monolayer MnSe with Unusual Atomic Structure and Antiferromagnetic Ordering, ACS Nano, DOI: 10.1021/acsnano.1c05532, (2021).

[6] Yung-Chang Lin, Jeyakumar Karthikeyan, Yao-Pang Chang, Shisheng Li, Silvan Kretschmer, Hannu-Pekka Komsa, Po-Wen Chiu, Arkady V Krasheninnikov, Kazu Suenaga, Formation of Highly Doped Nanostripes in 2D Transition Metal Dichalcogenides via a Dislocation Climb Mechanism, Advanced Materials, 33, 12, 2007819, (2021).

[7] J. Karthikeyan, H. P. Komsa, M. Batzill, A. V. Krasheninnikov, Which Transition Metal Atoms can be Embedded into Two-dimensional Molybdenum Dichalcogenides and Add Magnetism?, Nano Letters 19 (7), 4581-4587, (2019).

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[9] K. O. Ogunniran, G. Murugadoss, R. Thangamuthu, J. Karthikeyan, P. Murugan, Integration of phenylammoniumiodide (PAI) as a surface coating molecule towards ambient stable MAPbI3 perovskite for solar cell application, Solar Energy Materials and Solar Cells, 191, 316-328, (2019).

[10] V Parthiban, Balasubramaniam Bhuvaneshwari, J Karthikeyan, P Murugan, AK Sahu, Fluorine-enriched mesoporous carbon as efficient oxygen reduction catalyst: understanding the defects in porous matrix and fuel cell applications, Nanoscale Advances, 1 (12), 4926-4937, (2019).

[11] T. K. Bijoy, J. Karthikeyan, P. Murugan, Computational Approach To Reveal the Structural Stability and Electronic Properties of Lithiated M/CNT (M= Si, Ge) Nanocomposites as Anodes for Lithium-Ion Batteries, ACS Omega 4 (2), 4153-4160, (2019).

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[13] J. Karthikeyan, Y. S. Ranawat, P. Murugan, Vijay Kumar, Borophene Layers on Al(111) Surface –The Finding of a Borophene Layer with hexagonal Double Chain and B9 Nonagons from Ab initio Calculations, Nanoscale, 10, 17198-17205, (2018).

[14] S. Sekar, J. G. Muller, J. Karthikeyan, P. Murugan, N. Lakshminarasimhan, Unveiling the multifunctional roles of hitherto known capping ligand oleic acid as blue emitter and sensitizer in tuning the emission colour to white in red-emitting phosphors, Physical Chemistry Chemical Physics 20 (28), 19087-19097, (2018).

[15] T. K. Bijoy, J. Karthikeyan, P. Murugan, Exploring the mechanism of spontaneous and lithium-assisted graphitic phase formation in SiC nanocrystallites of a high capacity Li-ion battery anode, The Journal of Physical Chemistry C 121 (28), 15106-15113, (2018).

[16] S. M. Senthil Kumar, K. Selvakumar, J. Karthikeyan, R. Thangamuthu, P. Murugan, P. Rajput, S. N. Jha, D. Bhattacharyya, and N. Navascues, Manifestation of Concealed Defects in MoS_2 Nanospheres for Efficient and Durable Electrocatalytic Hydrogen Evolution Reaction, Chemistry Select, 2, 4667-4672, (2017).

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[18] Iflah Laraib[$], J. Karthikeyan[$], P. Murugan, First Principles Modeling of Mo_6S_9 Nanowire via Condensation of Mo_4S_6 Clusters and Effect of Iodine Doping on Structural and Electronic Properties. Physical Chemistry Chemical Physics, 18, 5471-5476, (2016). [$ Equal Contribution]

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[23] J.G. Muller, J. Karthikeyan, P. Murugan, N. Lakshminarasimhan, Influence of Structural Polymorphs on Tunable White Light Generation from Orange-Red-Emitting $BiPO_4:Eu^{3+}$ Phosphor by Surface Modification, The Journal of Physical Chemistry C, 118, 19308-19314, (2014).
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Major Research Projects in Progress and Completed:

1. Project at Rajiv Gandhi Institute of Petroleum Technology, Jais

Atomic clusters of transition metal atoms are suitable catalysts due to their high surface energy. However, they are stable only when some capping atoms protect their surface. The capping atoms are usually some halogens or/and chalcogens or small molecules. For many transition metal (almost for all) atoms, octahedron-shaped clusters are stable in protected form. Interestingly, for some transition metals (Sc, Y, Nb, Mo, Ta, W, and Re), the capped octahedron clusters assemble into one-, two-, and three-dimensional structures called cluster compounds. Also, they are known as metal-rich compounds. In such compounds, the octahedrons connect in different fashions. The capping atoms can combine two or many corners, edges, and faces of octahedrons, without forming additional metal-metal bonds between the octahedron clusters. For example, iodine atoms connect the Mo_6 octahedron in the $Mo_6S_{9-x}I_x$ nanowire structure. Otherwise, the octahedron can share one or many of its corners, edges, and faces through inter-cluster metal-metal bonds. For example, in two-dimensional MXenes layers, the metal octahedrons share three faces with three adjoining octahedrons. Consequently, the structure and dimensionality of these cluster frameworks are unique for any combination of transition metal atoms and capping atoms. Does this answer the questions: (1) Which combination of transition metals and chalcogens or halogens are the metal-rich compounds dynamically stable in one-, two-, and three- structures? What would be the structure of such metal-rich halides and chalcogenides compounds? (3) What are their structural, electronic, magnetic, and electrochemical properties? and (4) Will they be useful in energy storage and conversion application? This project will bring out the answers by employing high-throughput density functional calculations to study different cluster frameworks of octahedron clusters of all transition metal atoms. They will be tested for energy storage (sodium and potassium ion batteries) and energy conversion (hydrogen generation through hydrogen reduction reaction).

2. Project at Aalto University: (as Post Doctoral Fellow)

Metal Impurities resulted from Post-Modification Process on Two-Dimensional Materials

Two-dimensional (2D) materials in which the constituent atoms chemically(strongly) bonded in two directions and physically (very weakly) in the third direction rule the world of materials due to their "surface-only" driven properties that are not available in bulk counterparts. Such properties of these 2D materials are extremely sensitive to the number of layers stacked, stacking order, the relative orientation of layers, and chemical doping. From the perspective of a materials scientist, it is possible to tune or combine the physical and chemical properties of any material is possible by physical or chemical means. Chemical modification techniques are easy to engineer a material's properties, especially in 2D dichalcogenide materials; heteroatoms can dope metal and chalcogen atoms. This doping can be done during the growth of the layer(in situ) or after the growth of layers(post-growth). The post-growth process is mainly feasible only for the di-selenides and -tellurides layer; for example, Vanadium, Titanium, and Molybdenum impurities are introduced in $MoSe_2$ and $MoTe_2$ layers. I used high-throughput DFT calculations to understand the atomic structure and electronic and magnetic properties of all transition metal impurities in MoX_2 (X = S, Se, and Te) layers.

3. Project at CSIR-CECRI: (as Junior/Senior Research Fellow)

2.1 Project on Mo-S compounds (Ph.D., Thesis Work)

In this project, I used density-functional theory calculations to understand the electrochemical properties of Mo-S nanostructures. First, we investigated the magnetism in single-layer MoS_2 and small MoS_{2+x} clusters. Our study revealed the tailoring of magnetic properties under mechanical strain. Further, we investigated Mo-S nanowires to understand their structural and electronic properties upon iodine doping. For the first time, we reported that valence electron concentration plays a vital role in determining the structural stability and electronic properties of $Mo_6S_{9-x}I_x$ nanowires. Now I am extending the same concept to other metal chalcogenide nanowires. The structure of the Mo_6S_9 nanowire needed to be understood in its pristine form (without iodine). We have shown that a Mo_4 tetrahedron is more stable than a Mo_6 octahedron for forming nanowires with the Mo_6S_9 stoichiometry. We also studied MoS_2 single layers in hexagonal and tetragonal forms. We studied the effect of curvature on the catalytic properties of MoS_2 nanoparticles formed by Dr. S.M. Senthil Kumar's research group at CECRI. They observed that the MoS_2 in sphere-like morphologies are better catalysts for hydrogen evolution reactions than other morphologies. Our calculations played a crucial role in explaining the origin of this catalytic efficiency. Thus, we demonstrated the feasibility of concealed defects in the curved MoS_2 single layer. We proved these hidden defects have a better catalytic performance than edge sites and point defects. Now we are extending this work to

understand the effect of the radius of curvature of MoS_2 nanospheres on their catalytic properties. I am also working on large-size planar gold clusters stabilized on MoS_2 single layers to explore their structural, electronic, and catalytic properties.

2.2 Project on $BiPO_4:Eu^{3+}$ phosphor compounds

The main aim of the project was to produce white-light-emitting materials at a low cost. This project was carried out with Dr. N. Lakshminarasimhan's research group to understand the effect of different polymorphs of the host material $BiPO_4$ and its surface modification on the electronic energy transfer from sensitizer to the light emitter (Eu^{3+} dopant). Our DFT calculations proved a weak interaction between the monoclinic $BiPO_4$ and oleic acid, which acts as a sensitizer. The interaction was more vital for the hexagonal phase of $BiPO_4$, which facilitated the energy transfer from oleic acid to the Eu^{3+} ion. The electronic structure calculations explained the role of partially filled mid-gap states in hexagonal $BiPO_4$ for better electronic energy transfer.

Scientific Achievements/Discoveries

✓ 24 papers published in peer-reviewed journals.

✓ High throughput DFT calculations to understand post-modified molybdenum dichalcogenides.

✓ Explained the tuneable edge magnetism in MoS_2 nanoparticles.

✓ For the first time, reported the effect of the valence electron concentration on structural stability and electronic properties of $Mo_6S_{9-x}I_x$ nanowires.

✓ Found the best atomistic model for $Mo_6S_{9-x}I_x$ nanowires, in contrast to models previously reported by many groups. Ultimately, the electronic properties of our atomistic model are well corroborated by experimental reports.

✓ Proposed the formation of concealed defects in MoS_2 single layers and their catalytic properties for hydrogen evolution reaction.

✓ Demonstrated stabilization of large-size planar gold clusters on MoS_2 single layers without doping or defects [Unpublished Result].

Research Grants Awarded

➢ DST-Inspire Faculty Award (Award No. DST/INSPIRE/04/2019/000283). This award carries a monthly salary of Rs. 1.25 Laks and a yearly project grant of Rs. 7,00,000 for the next five years (2020-2025).

➢ CSIR selected me for the Senior Research Fellowship (Grant No. 31/20(145)/2015-EMRI). This fellowship covers a monthly stipend of Rs. 28,000 with a 10% housing rent allowance and a yearly contingency grant of Rs. 20,000 for three years (2015-2018).

➢ Department of Science and Technology, Science and Engineering Research Board awarded me an international travel grant to participate in the IUMRS-ICEM-2016 conference held in Singapore. (Grant No. ITS/1366/201617). Rs. 55,000 was allocated for his travel.

Academic Awards Received

- Selected as DST-Inspire Faculty for five years (2020-2025) to establish an independent research group in India.
- Selected as CSIR-Senior Research Fellow (SRF) for three years (2015 – 2018) to continue my research at CSIR-Central Electrochemical Research Institute, India.
- Best Poster Award at the International Conference on Electronic Materials-2016, organized by the International Union of Materials Research Society in Singapore.
- Best Poster Award at the International Conference on Advanced Materials for Power Engineering-2015 conference held in India.
- Best Poster Award at the Winter School on "Frontier in Materials Science" – 2014 in India.
- Best Poster Award at the IUMRS- International Conference on Advanced Materials – 2013 held in India.
- Qualified in Graduate Aptitude Test for Engineering (GATE) exam – 2011 and joined as Junior Research Fellow (JRF) at CSIR- Central Electrochemical Research Institute, India.
- B.Sc., Physics Gold Medal (College Level) – 2009.

References

1. **Dr. P. Murugan**, Senior Scientist, CSIR-Central Electrochemical Research Institute, India, (e-mail: murugan@cecri.res.in).
2. **Prof. Vijay Kumar**, Founder President and Principal Scientist, Dr. Vijay Kumar Foundation, Haryana, India (e-mail: vijay.kumar@snu.edu.in).
3. **Dr. Hannu Pekka Komsa,** Microelectronics Research Unit, Faculty of Information Technology and Electrical Engineering, University of Oulu, FI-90014, Oulu, Finland (e-mail: Hannu-Pekka.Komsa@oulu.fi)

PERSONAL PROFILE

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