

# CURRICULUM VITAE

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Professor

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## Summary of Research Interests

• Condensed matter theory • Quantum ab-initio theory for real materials • Physics and chemistry of hydrogen interactions with materials • Hydrogen generation and storage • Mechanical, structural, electronics, magnetism, and conductivity of novel nanostructures including graphene, nanowires, nanotubes and nanoclusters • Theory of defects, impurities, doping and diffusion in solids, • Thermoelectric materials, • Li ion batteries, shape memory alloys, • Machine learning, • Heterogeneous catalysis, • High throughput approach to design of functional materials

## Education

### ■ PhD in Computational Materials Science

[Institute for Materials Research](#), Tohoku University, Sendai, Japan ..... 09/2004

### ■ MSc in Physics

[Indian Institute of Technology Delhi](#), New Delhi, India ..... 05/2001

### ■ BSc Physics Honors

[St. Xaviers College](#), Ranchi University, Ranchi, India ..... 12/1998

## Honors and Awards

- JSPS Postdoctoral Research Fellowship, 2004-2006
- Monbukagakashu (MEXT) Graduate Research Fellowship, 2001-2004
- Materials Research Society of India Medal, 2014
- Distinguished lectureship award of chemical society of Japan, 2020
- JSPS invitation fellowship, 2020

## Professional Experience

### ■ [Materials Research Centre, Indian Institute of Science](#), Bangalore, India

Professor ..... 06/2021 – Present

- **Materials Research Centre, Indian Institute of Science**, Bangalore, India  
Associate Professor ..... 05/2016 – 06/2021
- **Materials Research Centre, Indian Institute of Science**, Bangalore, India  
Assistant Professor ..... 06/2010 – 05/2016
- **Department of Materials Science and Nanoengineering, Rice University**, Houston, Texas, USA  
Adjunct Associate Professor ..... 06/2016 – Present
- **Department of Materials Science and Nanoengineering, Rice University**, Houston, Texas, USA  
Adjunct Assistant Professor ..... 06/2010 – 05/2016
- **Department of Mechanical Engineering and Materials Science, Rice University**, Houston, Texas, USA  
Postdoctoral Research Associate ..... 08/2007 – 05/2010
- **Materials Department, University of California Santa Barbara**, California, USA  
Postdoctoral Research Scholar ..... 03/2006 – 07/2007
- **Institute for Materials Research, Tohoku University**, Sendai, Japan  
JSPS Postdoctoral Fellow ..... 10/2004 – 02/2006  
Graduate Student ..... 10/2001 – 09/2004
- **Indian Institute of Technology Delhi**, New Delhi, India  
Research Assistant ..... 05/2001 – 08/2001

## Editorial Board Member

- Editorial Board Member, *J. Phys: Materials* 09/2018 – Present
- Editorial Board Member, *Scientific Reports*, 06/2015 – Present
- Guest Editor, *International Journal of Hydrogen Energy*, 2015-2016

## Selected Presentations

- **Invited presentations**
  1. “Accelerated Discovery of Novel Materials using Machine Learning” Density Functional Theory (DFT) Modelling and Machine Learning in Chemistry Ramaiah University of Applied Sciences, Bangalore, April 12<sup>th</sup>, 2023
  2. “Accelerated Discovery of Novel Materials using Machine Learning” Instructional School on AI and ML for Researchers, IISc, Bangalore, March 25<sup>th</sup>, 2023.
  3. “Accelerated Discovery of Novel Materials using Machine Learning” Advances in Low-dimensional Materials for Optoelectronic and Nano Devices (ALMOND 2023), March 3<sup>rd</sup>, 2023.
  4. “Accelerated Discovery of Novel Materials using Machine Learning” International Workshop on Nano-Engineered Materials, IISER Trivandrum January 5<sup>th</sup>, 2023.
  5. “Database to Knowledge Base” Pontificia Universidad Católica de Chile, 22<sup>nd</sup> August 2022.
  6. “Accelerated Discovery of Novel Materials using Machine Learning” Tokyo University, 29<sup>th</sup> July 2022.

7. "Accelerated Discovery of Novel Materials using Machine Learning" Osaka University 22<sup>nd</sup> July 2022.
8. "Machine learning assisted search for knowledge and insights into materials properties" Tokyo University of Science and Technology, 20<sup>th</sup> July 2022.
9. "Role of point defects in making semi insulating GaN" Tohoku University, 12<sup>th</sup> July 2022.
10. "Data Assisted Discovery of Novel Materials" 23<sup>rd</sup> June 2022, Cluster Research Laboratory, Toyota Technological Institute
11. "ML Assisted Knowledge Discovery", 24<sup>th</sup> March 2022, ICMG-II, SRM University AP, India.
12. "ML Assisted Discovery of Novel Materials", 2<sup>nd</sup> March 2022, National Computerized Maintenance Management System, India.
13. "Machine learning approach for alloy modelling", February 2021, Faculty development program, NIT Warangal, India
14. "AI assisted discovery of materials to knowledge discovery", October 2021, Cambridge IISc workshop, Indian Institute of Science, India.
15. "ML assisted discovery of novel materials" September 2021, CTTC-BARC, Bhabha Atomic Research Centre (BARC), India.
16. "Data driven materials science" February 2021, IISc WIN Workshop, Bangalore, India.
17. "ML assisted discovery of novel materials", October 2021, University of south Florida, Tampa, USA.
18. "Data assisted insights to overcome challenges associated to thermoelectric" March 2021, Keynote lecture, Chemical Society of Japan Annual Meeting.
19. "Data driven insights into materials design", December 2021, MRS Fall Meeting and Exhibit, Boston, Massachusetts.
20. "ML driven approach to overcome challenges associated with thermoelectric", 23<sup>rd</sup> December 2021, Thermoelectric theme, Third Indian Materials Conclave (IndMac) and 32<sup>nd</sup> Annual General Meeting of MRSI.
21. "Data-assisted Insights to Materials Design", July 2021, International Conference on "Materials for Humanity (MH 21)" Singapore.
22. "Data-assisted Insights to Overcome Challenges Associated with Thermoelectrics", July 2021, The Twelfth International Conference on the Science and Technology for Advanced Ceramics (STAC12), Tokyo Tech, Tokyo.
23. "ML Assisted Discovery of Novel Materials with Targeted Properties" February 2021, 6<sup>th</sup> International Conference on Nanoscience and Nanotechnology, ACCMS and SRMIST.
24. "Application of Machine Learning in Materials Science and Engineering" December 2020, Webinar, Evolution of Electronic Structure Theory and Experimental Realization, Jointly organized by SRMIST KTR (India), IIT Madras (India) and Uppsala University (Sweden).
25. "Application of Machine Learning and First-principles in Ni-based Alloys" December 2020, Webinar, Indian Academy of Sciences and IISc workshop, Orange County, Coorg.
26. "Strain induced tuning of physical properties of materials" Webinar, MRS Fall Meeting, USA.
27. "Accelerated Discovery to Knowledge using Machine Learning" 10<sup>th</sup> October 2020, Webinar, ThoughtWorks E4R Seminar, Bangalore.
28. "Unravelling the role of bonding chemistry in connecting electronic and thermal transport by machine learning" 17<sup>th</sup> September 2020, SISPAD2020 Workshop, Kobe, Japan.

29. "Data-driven Materials Science: Accelerated Discovery to Knowledge" 17<sup>th</sup> August 2020, Webinar, Tata Steel Limited, Jamshedpur.
30. "Data-driven Materials Science: Accelerated Discovery to Knowledge" 28<sup>th</sup> May 2020, Webinar Materials Simulation: A Virtual Guided Tour, IIT Delhi, New Delhi.
31. "Data-driven Accurate Prediction of Functional Properties of Materials", 27-29<sup>th</sup>, May 2020, 2020, 18<sup>th</sup> (National) Conference of the Society of Nano Science and Technology, Japan.
32. "Data Driven Material Science for Electronic Materials" 24<sup>th</sup> May 2020, Webinar, AIMD Workshop, IIT Bombay, Mumbai.
33. "Accelerated Discovery of Functional Materials using Machine Learning Combined with High Throughput Screening" Award Lecture, March 22-25<sup>th</sup>, 2020, Tokyo University of Science, Chiba, Japan.
34. "Accelerating the Discovery of Functional Materials by Machine Learning" 2<sup>nd</sup> March 2020, (Virtual) 7<sup>th</sup> Asian Materials Data Symposium, Awaji Island, Japan.
35. "Machine Learning In Materials Science" 6<sup>th</sup> March 2020, Faculty Development Program, SRM University Chennai.
36. "Combined High-Throughput and Machine learning Approach for Prediction of Lattice Thermal Conductivity" 5- 7<sup>th</sup> February 2020, ACCMS: International Conference on Materials Genome (ICMG-2020), SRM University, Amravathi.
37. "Rational design of high-performance thermoelectric materials" 12-15<sup>th</sup> Feb 2019, The First Indian Materials Conclave held at the Indian Institute of Science, Bangalore
38. "Accelerated Development of High Performance Materials using Machine Learning" 6<sup>th</sup> Feb 2019, BARC, Mumbai
39. "A Machine Learning Based Approach for Accelerated Discovery of Materials for Energy" 12-14<sup>th</sup> December 2018, Modelling and Simulations of Materials for Energy and the Environment, JNCASR, Bangalore
40. "Metal-semiconductor classification and prediction of accurate bandgap of functionalized MXene using machine learning"
41. "Accelerated development of high performance materials using artificial intelligence" 20<sup>th</sup> December 2018, DMRL, Hyderabad, October 30<sup>th</sup> to November 2<sup>nd</sup> 2018, The International Conference on Emerging Advanced Nanomaterials 2018 (ICEAN-2018), Newcastle, Australia
42. "Prediction of Accurate Bandgap of Functionalized MXene using Machine Learning Based Models" 4-9<sup>th</sup> October 2018, International Workshop on Materials Genome (IWMG2018), Shanghai University, Shanghai, China
43. "Addressing Challenges in Development of Efficient Thermoelectric Materials" 23 August 2018, ETRI Daejeon Korea
44. "Estimation of Accurate Bandgap of Functionalized MXene using Statistical Learning" 19-24<sup>th</sup> August, 2018 IUMRS-ICEM, Daejeon, Korea
45. "MXene : A promising 2D material for energy applications" 7<sup>th</sup> July 2018, Indo-US Joint Center: "Light Induced Energy Technologies: Utilizing Promizing 2D Nanomaterials (LITE UP 2D) Kick-off meeting, IISER Thiruvananthapuram.
46. "Accelerated Development of High Performance Materials using Artificial Intelligence" 28<sup>th</sup> June 2018, DMRL, Hyderabad.

47. "Accelerated Development of High Performance Materials using Machine Learning" 10<sup>th</sup> August 2018, Pre-workshop on ICME Approaches to Innovation in Biomedical Implants, IISc Bangalore
48. "Addressing Challenges in Development of Efficient Thermoelectric Materials" 14-17<sup>th</sup> April 2018, 2018 International Conference on Advanced Energy Materials (AEM 2018), Hefei, China
49. "Frontiers in Materials/Chemical Informatics and Multiscale modeling" Division of Chemical Sciences Meeting, 6<sup>th</sup> January 2018, Bangalore.
50. "Rational Design of Efficient Thermoelectric Materials" 26-30<sup>th</sup> December, 62<sup>nd</sup> DAE Solid State Physics Symposium (DAE SSPS-2017), Mumbai.
51. "Machine-Learning Assisted Accurate Band Gap Predictions of Functionalized MXene" 17-19<sup>th</sup> December, 2017, ACCMS VO11 Sendai Japan.
52. "Machine-Learning Assisted Accurate Band Gap Predictions of Functionalized MXene" 11-14<sup>th</sup> December 2017, Japan-India YNU Symposium 2017 on Emerging Materials & Systems for Green and Life Innovations
53. "Development of Catalysts for a Clean Energy and a Sustainable Environment" 11<sup>th</sup> Dec 2017, Seminar at Cluster Lab. Toyota Institute of Technology, Tokyo, Japan.
54. "Rational design of high-performance thermoelectric materials" 31<sup>st</sup> October to 3<sup>rd</sup> November, Recent Trends in Condensed Matter Physics, 30 October to 3<sup>rd</sup> November 2017, Bose Institute, Kolkata
55. "Strain-Induced Electronic Phase Changes in Layered Materials" 17-21<sup>st</sup> April 2017 MRS Spring Meeting Phoenix, USA
56. "High throughput design of efficient thermoelectric materials" 19-21<sup>st</sup>, December, 2016, ACCMS VO11 Sendai Japan.
57. "Search for Descriptors for Computational Design of Efficient Thermoelectric Materials" 14-20<sup>th</sup> December, 2016, JSPS-DST Asian Academic Seminar 2016, Tokyo, Japan.
58. "Outlook and Challenges for Hydrogen Storage via Kubas Interaction" IUMRS-ICYRAM 2016, 11-15<sup>th</sup> December, 2016, Bangalore, India.
59. "Principles for rational design of high-performance thermoelectric materials" 5-9<sup>th</sup> December, 2016, Winter School JNCASR, Bangalore, India.
60. "Challenges in exploiting the Kubas Interaction in Hydrogen Storage" 21-24<sup>th</sup> September, 2016, ACCMS SRM 2016, Chennai India.
61. "Computational Design of Efficient Thermoelectric Materials" 4-8<sup>th</sup> July, 2016, IUMR-ICEM Singapore.
62. "Computational Materials Science at MRC" 21<sup>st</sup> Dec 2015, IISc-IKIST Joint workshop on Advanced Materials and Modelling, Bangalore, India.
63. "Bimetallic Catalyst: A solution to Pt-Poisoning-Free CO Oxidation" 15<sup>th</sup> Dec 2015, Seminar at Physics Dept. Yokohama National University, Japan
64. "Pt-Poisoning-Free Efficient CO Oxidation on Supported Pt<sub>3</sub>Co Catalyst" 15<sup>th</sup> Dec 2015, Seminar at Cluster Lab. Toyota Institute of Technology, Tokyo, Japan.
65. "Applications of Computational Materials Science" 10<sup>th</sup> Dec 2015, Seminar at National College of Technology, Akita Japan
66. "Addressing the Challenges in Designing Efficient Thermoelectric Materials" 1-3<sup>rd</sup> Nov 2015, ACCMS-VO 10, Sendai, Japan (**Keynote Lecture**)

67. "Reversible Tuning of "Electronic Structure" of Semiconducting Transition Metal Dichalcogenides" 16<sup>th</sup> September 2015, Seminar at ISER Trivandrum, India
68. "Strain-induced phenomena in layered materials" 27-30<sup>th</sup> July 2015, IEEE Nano 2015, Rome, Italy.
69. "Efficient Hydrogen Storage on Free-standing  $Ti_3B$  and  $Ti_3@BC_3$ " ANM2015, 20 - 22<sup>th</sup> July 2015, Aveiro, Portugal.
70. "Strain induced tuning of electronic and thermoelectric properties of TMDs" ACCMS VO10, 20 - 22<sup>nd</sup> December 2014, Okinawa, Japan.
71. "Pressure-induced Semiconductor to Metal Transition in  $MoS_2$ : Prediction to Reality" ENGE 2014 17-19<sup>th</sup> November 2014 Jeju Island South Korea
72. "Reversible Tuning of Electronic Structure of Semiconducting Transition Metal Dichalcogenides" Institute Seminar at SN Bose National Centre for Basic Sciences, 19<sup>th</sup> September 2014, Kolkata, India.
73. "Density Functional Theory: Basic Principles and Applications" Application of Numerical Techniques in Materials Research, RV College of Engineering 10-12<sup>th</sup> of July 2014, Banaglore India.
74. "Tuning Electronic Properties of Semiconducting Transition Metal Dichalcogenides" Department Seminar at Department of Electrical Engineering, UT Austin, 13<sup>th</sup> of June 2014, Austin USA.
75. "Tuning Electronic Properties of Semiconducting Transition Metal Dichalcogenides" Molecular Simulations of Fluids at Interfaces, IISc, 24<sup>th</sup> of March, Banaglore India.
76. "Tuning Electronic Properties of Semiconducting Transition Metal Dichalcogenides" Award Lecture, MRSI AGM 13<sup>th</sup> February 2014 IISc Banaglore.
77. "Tuning Electronic Properties of Semiconducting Transition Metal Dichalcogenides" US-India Tunable Materials Technical Exchange Meeting, Dayton, Ohio, USA, on 25-27<sup>th</sup> March 2014.
78. "Designing New Functional Materials Using First Principles Calculations" NRC-M Winter Workshop on Integrated Computational Materials Engineering, December 2013, Bangalore, India
79. "Tuning of Electronic Properties of Semiconducting Bilayer Transition Metal Dichalcogenides by Applying Normal Pressure" Nanotechnology based innovation for Environmental, Energy and Biomedical Applications" IISC, December 2013, Bangalore, India
80. "Role of defect transition level in tuning the thermoelectric properties of doped  $CrSi_2$ " Advanced Lecture at Toyota Institute of Technology, December 2013, Tokyo, Japan
81. "Examples of Materials Design by First Principles Methods" Advanced Lecture at Akita National College of Technology, December 2013, Akita, Japan
82. "New Insights into Designing Metallacarborane Based Room Temperature Hydrogen Storage Media" Special seminar at Kawazoe Group, December 2013 Sendai, Japan
83. "Graphitic Materials as Promising Hydrogen and Li Storage Media" 1st Workshop on Promising Graphitic Anode Materials for Li-ion Battery, November 2013, Seoul, Korea
84. "Origin of enhanced thermoelectric properties of doped  $CrSi_2$ " The Seventh General Meeting of ACCMS-VO 7-9v November 2013, Sendai, Japan
85. "Graphitic Materials as Promising Hydrogen Storage Media" 1st TUE-Workshop, SSCU, IISc, 20-23<sup>rd</sup> Aug 2013, Bangalore, India.
86. "Normal Pressure Induced Bandgap Tuning of 2D-Semiconducting Transition Metal Dichalcogenides" ACCMS-7, Suranaree University of Technology, 25-28<sup>th</sup> July 2013, Nakhon Ratchasima,

Thailand.

87. "A New Insight in Designing Metallacarborane Based Hydrogen Storage Media" One Day Workshop on Gas Storage, Department of Chemical Engineering IISc, 29<sup>th</sup> April 2013, Bangalore, India.
88. "Normal Pressure Induced Band Gap Tuning of 2D-Materials" First National Conference on Mapping the Materials Genome Shiv Nadar University, 8-10<sup>th</sup> March 2013, Delhi, India.
89. "Interfaces in Graphitic Hybrid Materials" Science of Clusters, Nanoparticles and Nanoscale-Materials (SOCNAM) 4-7<sup>th</sup> March, 2013 Jaipur, India
90. "Mechanisms of Hydrogen Storage in Graphitic Materials by First Principles Calculations" International workshop on Computational Materials Design and Engineering (IWCMD) 8-10<sup>th</sup> February 2013, Jodhpur, India.
91. "Effect of Normal Strain on Electronic Properties of few layers of MoS<sub>2</sub>" Electronic Structure Approaches to atoms, molecules-clusters and solids meeting in UoH from 7-11<sup>th</sup> Jan 2013, Hyderabad, India.
92. "Contributions of electronic structure calculation to hydrogen storage" Seminar in Yokohama National University, 14<sup>th</sup> December 2012, Yokohama, Japan.
93. "Graphene and its functionalized derivatives: From electronics to energy" Seminar in Akita National College of Technology, 7<sup>th</sup> December 2012, Akita, Japan.
94. "Graphene: From Electronics to Energy" One Day Workshop at Osaka University, 28<sup>th</sup> November 2012, Osaka, Japan.
95. "Stress Induced Tuning of Band Gap in Bilayer Transition Metal Dichalcogenides" The Seventh General Meeting of ACCMS-VO 23-25<sup>th</sup> November 2012, Sendai, Japan.
96. "Challenges in Hydrogen Energy: Storage Media" National Conference on Chemistry Challenges & Opportunities (NCCCO-2012), 16-18<sup>th</sup> Feb. 2012, Bangalore, India.
97. "Interfaces in Graphitic Materials" The Sixth General Meeting of ACCMS-VO 10-12<sup>th</sup> February 2012, Sendai, Japan.
98. "Graphene: From Electronics to Energy" Seminar in Reva Educational Institute of Engineering colleges, 12<sup>th</sup> November 2011, Bangalore, India.
99. "Application of electronic structure calculation in hydrogen storage" Frontiers of Electronic Structure Calculations and their Applications, 14-17<sup>th</sup> January 2011, Hyderabad, India.
100. "Hydrogen Energy: Challenges and Opportunities" Vision for Engineering Education in 2020, 8<sup>th</sup> January 2011, Bangalore, India.
101. "Digging Wells in Graphane to Mine Graphene Roads and Quantum Dots" The Fourth General Meeting of ACCMS-VO, 10-13<sup>th</sup> December 2010, Sendai, Japan.
102. "Interfaces and Patterns in Functionalized Graphene" Seminar in Theoretical Sciences Unit, JNCASR, 19<sup>th</sup> October 2010, Bangalore, India.
103. "H-Spillover through the catalyst saturation: A first principle study" The Fourth General Meeting of ACCMS-VO, 12-14<sup>th</sup> January 2010, Sendai, Japan.
104. "Graphene: hydrogen storage to electronics" MRC IISc, 16<sup>th</sup> of July 2009, Bangalore, India.
105. "Carbon nanostructures for molecular hydrogen confinement" ACS Meeting, 22-26<sup>th</sup> March 2009, Salt Lake City, USA.

106. "Catalyst as a spillover pump"  
HPC Users Workshop, 1<sup>st</sup> Oct 2008, Houston USA.
107. "Exploration of the structure-property relation at nanoscale: from clusters to nanowires"  
CECAM Workshop on Structural, electronic and transport properties of quantum wires, 9-12<sup>th</sup>  
June 2008, Lyon, France.
108. "Theoretical design, possibilities and challenges in applications of nanowires in electronics,  
sensing and optical devices"  
ICYS, 15<sup>th</sup> May 2007, Tsukuba, Japan.
109. "Stabilizing the silicon fullerene Si<sub>20</sub> by thorium encapsulation"  
Workshop on Nanoclusters, 11-12<sup>th</sup> May 2005, Sendai Japan.
110. "Cluster assembled metal encapsulated nanotubes of Silicon and Germanium"  
Particles 2004, 6-9<sup>th</sup> March 2004, Orlando FL USA.



# LIST OF PUBLICATIONS

## Research Articles

1. P. Pandey, M. Heczko, N. Khatavkar, N. Mazumder, A. Sharma., A. K. Singh, M. J. Mills, K. Chattopadhyay, On the faulting and twinning mediated strengthening and plasticity in a  $\gamma'$  strengthened CoNi-based superalloy at room temperature, [Acta Mater., 252, 118928 \(2023\)](#).
2. R. Ahmad, H. Yasumatsu, and A. K. Singh, Highly Efficient CO Oxidation on Atomically Thin Pt Plates Supported on Irreducible Si  $7\times 7$ , [J. Phys. Chem. C, 127, 4527 \(2023\)](#).
3. P. Kumbhakar, A. Parui, S. Dhakar, M. Paliwal, R. Behera, A. R. Singh Gautam, S. Roy, P. M. Ajayan, S. Sharma, A. K. Singh, C. S. Tiwary, Spontaneous Hydrogen Production using Gadolinium Telluride, [iScience, 26, 106510 \(2023\)](#).
4. R. Das, R. Paul, A. Parui, A. Shrotri, C. Atzori, K. A. Lomachenko, A. K. Singh, J. Mondal, S. C. Peter, Engineering the Charge Density on an  $\text{In}_{2.77}\text{S}_4$ /Porous Organic Polymer Hybrid Photocatalyst for  $\text{CO}_2$ -to-Ethylene Conversion Reaction, [J. Am. Chem. Soc., 145, 422 \(2023\)](#).
5. K. Das, R. Das, M. Riyaz, A. Parui, D. Bagchi, A. K. Singh, A. K. Singh, C. P. Vinod, S. C. Peter, Intrinsic Charge Polarization in  $\text{Bi}_{19}\text{S}_{27}\text{Cl}_3$  Nano Roads Promotes Selective C-C Coupling Reaction During Photoreduction of  $\text{CO}_2$  to Ethanol, [Adv. Mater., 35, 2205994 \(2022\)](#).
6. S. Swetlana, A. Rout, A. K. Singh, Machine Learning Assisted Interpretation of Creep and Fatigue Life in Titanium Alloys, [APL Machine Learning, 1, 016102 \(2023\)](#).
7. N. Khatavkar, and A. K. Singh, Highly interpretable machine learning framework for prediction of mechanical properties of nickel-based superalloys, [Phys. Rev. Materials, 6, 123603 \(2022\)](#).
8. P. Kumbhakar, A. Parui, R. S. Ambekar, M. Mukherjee, S. Siddique, N. M. Pugno, A. K. Singh, and C. S. Tiwary, Rain Energy Harvesting Using Atomically Thin Gadolinium Telluride Decorated 3D Printed Nanogenerator, [Adv. Sustain. Syst., 6, 2200296 \(2022\)](#).
9. P. Kumbhakar, A. Parui, R. S. Ambekar, M. Mukherjee, S. Siddique, N. M. Pugno, A. K. Singh, and C. S. Tiwary, Strain-Modulated Interlayer Charge and Energy Transfers in  $\text{MoS}_2/\text{WS}_2$  Heterobilayer, [ACS Appl. Mater. Interfaces, 14, 46841-46849 \(2022\)](#)
10. A. Parui, P. Srivastava, and A. K. Singh, Selective Reduction of  $\text{CO}_2$  on  $\text{Ti}_2\text{C}(\text{OH})_2$  MXene through Spontaneous Crossing of Transition States, [ACS Appl. Mater. Interfaces, 14, 40913-40920 \(2022\)](#)
11. R. Pathak, P. Dutta, A. Srivastava, D. Rawat, R. K. Gopal, A. K. Singh, A. Soni, and K. Biswas, Strong Anharmonicity-Induced Low Thermal Conductivity and High n-type Mobility in Topological Insulator  $\text{Bi}_{1.1}\text{Sb}_{0.9}\text{Te}_2\text{S}$ , [Angew. Chem. Int. Ed., 61, e202210783 \(2022\)](#)

12. M. Mukherjee, A. Srivastava, and A. K. Singh, Recent Advances in Designing Thermoelectric Materials, **J. Mater. Chem. C**, **10**, 12524-12555 (2022).
13. S. Chakraborty, S. Marappa, S. Agarwal, D. Bagchi, A. Rao, C. Vinod, S. Peter, A. K. Singh, and M. Eswaramoorthy, Improvement in oxygen evolution performance of NiFe layered double hydroxide grown in presence of 1T rich MoS<sub>2</sub>, **ACS Appl. Mater. Interfaces**, **14**, 31951 (2022)
14. P. V. Sarma, R. Nadarajan, R. Kumar, R. M. Patinharayil, N. Biju, S. Narayanan, G. Gao, C. S. Tiwary, M. Thalukulam, R. Kini, A. K. Singh, P. M. Ajayan and M. Shaijumon, Growth of Highly Crystalline Ultrathin Two-dimensional Selenene, **2D Mater.**, **9**, 045004 (2022).
15. A. Srivastava, M. Mukherjee, and A. K. Singh, Decoupled atomic contribution boosted high thermoelectric performance in mixed cation spinel oxides ACo<sub>2</sub>O<sub>4</sub>, **Appl. Phys. Lett.**, **120**, 243901 (2022).
16. M. Dey, S. Chowdhury, S. Kumar, and A. K. Singh, Quantum Confinement Effect on Defect Level of Hydrogen Doped Rutile VO<sub>2</sub> Nanowires, **J. Appl. Phys.**, **131**, 235702 (2022).
17. C. C. Gowda, A. Mathur, A. Parui, P. Kumbhakar, P. Pandey, S. Sharma, A. Chandra, A. K. Singh, A. Halder, C. S. Tiwary, Understanding the electrocatalysis OER and ORR activity of ultrathin spinel Mn<sub>3</sub>O<sub>4</sub>, **J. Ind. Eng. Chem.**, **113**, 153-160 (2022).
18. A. Singh, M. Dey, and A. K. Singh, Origin of layer-dependent electrical conductivity of transition metal dichalcogenides, **Phys. Rev. B**, **105**, 165430 (2022).
19. S. Agarwal, A. K. Singh, Electroreduction of CO<sub>2</sub> with Tunable Selectivity on Au-Pd Bimetallic Catalyst: A First Principle Study, **ACS Appl. Mater. Interfaces**, **14**, 11313-11321 (2022).
20. S. Shetty, M. Gayen, S. Agarwal, D. Chatterjee, A. K. Singh, N. Ravishankar, Tuning Catalytic Activity in Ultrathin Bimetallic Nanowires via Surface Segregation: Some Insights, **J. Phys. Chem. Lett.**, **13**, 770, 601776 (2022).
21. B. Sarkar, A. Parui, D. Das, A. K. Singh and K. K. Nanda, Interfacial electron transfer strategy to improve the hydrogen evolution catalysis of CrP heterostructure, **Small**, **18**, 2106139 (2022).
22. E. Rathore, R. Juneja, D. Sarkar, S. Roychowdhury, M. Kofu, K. Nakajima, A. K. Singh, and K. Biswas, Enhanced Covalency and Nanostructured Phonon Scattering Lead to High Thermoelectric Performance in n-type PbS, **Mater. Today Energy**, **24**, 100953 (2022).
23. H. Lee, J. H. Park, N. Maity, D. Kim, D. Jang, C. Kim, Y. G. Yoon, A. K. Singh, Y. Han, and S. G. Yoon, Diffusion-enhanced preferential growth of m-oriented GaN micro-domains on directly grown graphene with a large domain size on Ti/SiO<sub>2</sub>/Si(001), **Mater. Today Commun.**, **30**, 103113 (2022).
24. P. Upadhyay, N. Maity, R. Kumar, P. K. Barman, A. K. Singh, and P. K. Nayak, Layer parity dependent Raman-active modes and crystal symmetry in ReS<sub>2</sub>,

- Phys. Rev. B, 105, 045416, (2022).**
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