

**Present Status**

Dr. Sudip Chakraborty (Ph.D in Physics)

Reader F

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**DOB:** 15/05/1984

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**Academic Appointments and Degrees**

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- 5/2021 –** : Reader F, Harish-Chandra Research Institute (HRI) Allahabad, India
- 3/2019 – 4/2021** : Assistant Professor, Department of Physics, IIT Indore, India
- 2/2013–2/2019** : Forskare (Senior Researcher), Materials Theory Division  
Department of Physics and Astronomy, Uppsala University, Sweden
- 6/2013–7/2013** : Visiting Scientist, Department of Chemistry, University of Cambridge
- 2011 – 2013** : Max-Planck Postdoctoral Fellow, MPIE, Düsseldorf, Germany
- 2006 – 2011** : Junior Research Fellow(2006-08) & Senior Research Fellow(2008-11)  
Department of Atomic Energy (DAE- BARC) Fellowship,  
Bhabha Atomic Research Centre (BARC) & University of Pune, India
- Ph.D. Thesis** : BARC and University of Pune, India. ((**28<sup>th</sup> February, 2011**))
- Thesis Title** : Density Functional Theory Based Calculations of Different Properties  
of Semiconductor Quantum Dots
- M.Sc.(Physics) 2006:** Department of Physics, University of Pune, India
- B.Sc.(Physics) 2004:** R. K. Mission College, Narendrapur, Calcutta University, India

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**Academic Awards and Honours**

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- Rising Star Award by ACS Materials Au among 300+ world-wide nominations, as the only recipient from India (**2022**).
- TCT Visiting Scientist Award, Singapore (**40,000 SEK**), **2016**.
- Carl-Tryggers Fellowship, Uppsala University, Sweden, **2013**.
- Max Planck Post Doctoral Fellowship, MPIE, Düsseldorf, Germany, **2011**.
- Senior (**2008**) and Junior (**2006**) Research Fellowship, Department of Atomic Energy (DAE-BARC), Govt. of India

- Dr. Gokhale Scholarship, 1<sup>st</sup> year (top 3), M. Sc, University of Pune, **2005**.
- Ranked 2<sup>nd</sup> (UGC Master Degree Fellow) in All India Entrance, Pune University, **2004**

### Project Grants

- 1. 2015 – 2017: Co-principal Investigator (60,000,00 INR)** Swedish Research Links (VR-SIDA) “Tunable catalytic properties of novel materials for renewable energy”
- 2. 2020 – 2023: Co-principal Investigator (68,000,00 INR)** Indo-Swedish Research Funding on “Rational Design of Transition Metal Based Nanoalloys and Two-Dimensional Materials for Direct Conversion of CO<sub>2</sub> into Gasoline Fuel”
- 3. July, 2020:** International Visiting Faculty Funding in Quantum Matter and Materials Cluster, University of Cologne, Germany
- 4. October, 2020:** DST-SERB-SRG (Starting Grant) as PI (Principal Investigator), (Amount: 31,39,000 INR)
- 5. November, 2020:** DST-SERB-CRG (Core Grant) as co-PI (co-Principal Investigator) (Amount: 65,00,000 INR).
- 6. March, 2021:** DST-NSM (National Supercomputing Mission) as PI (Principal Investigator) (Amount: 35,00,000 INR)
- 7. June, 2022:** DST Solar Challenge Award (Consortium Project of worth 650 Lacs INR: TIFR Hyderabad, HRI, IIT Bombay, IISER Berhampur)

### Research Supervision

I am leading my research group, Materials Theory for Energy Scavenging (MATES) Lab, in Physics Division, HRI Allahabad consisting of 6 Ph.D and 4 Postdoctoral Fellows.

#### **1. Supervision of Ph.D., Masters and Postdoctoral Fellows**

**A. Ph.D. Students (Ongoing): 6 as Supervisor + 1 as Co-supervisor**

**Ph.D (Completed): 4 as Co-supervisor**

**B. Postdoc Fellows: 5 (Ongoing) + 4 (Completed)**

**C. M.Sc./M.S/Project Students: 4 (Completed) + 6 (ongoing)**

**Current Ph.D. Students:** (i) Ms. Jagjit Kaur, (ii) Ms. Manasa G.B., (iii) Mr. Ponnappa K. P, (iv) Mr. Dharendra Kumar, (v) Mr. Arijeet Sarangi, (vi) Ms. Prajna Parimita Mohanty (as Co-Supervisor), (vii) Sankalpa Bora (DST-JRF)

**Current Postdoc Fellows:** (i) Dr. Shilendra Sharma, (ii) Dr. Swapnil Deshpande, (iii) Dr. Vanshree Parey, (iv) Dr. Muskan Nabi (with Dr. Tisita Das), (v) Dr. Pradhi Srivastava (jointly with Prof. Ravi Kumar)

**Current JRF/Masters/Long Term Project Students:** (i) Ayushi Tripathi, (ii) Taranga Borgohain, (iii) Rajib Sarkar (Joint M.S. Thesis, HRI+IISER-Kolkata), (iv) Dilip Sasmal (as Co-Supervisor)

**Previous Postdoc Fellows:** (i) Dr. Pushkar Mishra, (ii) Dr. Showkat Mir, (iii) Dr. Ranjini Sarkar, (iv) Dr. Shalini Tomar

**Previous Ph.D. Students:** 4 (Officially co-supervised in Materials Theory Division, Uppsala University with Prof. Rajeev Ahuja) (i) Dr. Amitava Banerjee (8/2014 - 2/2019), (ii) Dr. Vivekananda Shukla (9/2014 - 3/2019), (iii) Dr. Teeraphat Watcharatharapong (10/2014 - 5/2019), (iv) Dr. John Wårnä (10/2014 - 5/2019)

**Previous Masters Students:** (i) Mr. Jeevan Kumavat, (ii) Mr. Priyanka Yadav, (iii) Mr. Vardhman Diwadi, (iv) Mr. Diwakar Singh, (v) Pratik Aher, (vi) Ankit Bansal (Joint M.S. Thesis, HRI+IIT Madras)

**Previous Visiting Ph.D Students:** (i) Dr. Tae Amolozo (2013-2014), (ii) Dr. Jonas Anversa (2013-2014), (iii) Dr. Caroline Rupp (2013-2014), (iv) Dr. Mailing Berwanger (2014-2015), (v) Dr. Rosley Almeida (2016), (vi) Dr. Abera Abraha (2016), (vii) Dr. Atanfu (2016), (viii) Dr. Kelthoum Klää (2017), (ix) Dr. Zeleke Deressa (2018)

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### **Scientific Activity and Organization**

#### **1. Scientific Editor:**

1. Editorial Board Member, Journal of Physical Chemistry A/B/C (ACS)
2. Editorial Board Member, Electronic Structure, Institute of Physics (IOP)
3. Editorial Board Member, Energy Advances, Royal Society of Chemistry (RSC)
4. Editorial Board Member, Chemistry of Inorganic Materials, Elsevier
5. Editorial Board Member, Graphene and 2D Materials, Springer
6. Lead Guest Editor in Euro. Phys. J. ST (EPJST) with Prof. Chennupati Jagadish

#### **2. Scientific Reviewer:**

**ACS:** JACS, ACS Nano, Nano Letters, Chem.Mat., ACS Energy Letters, JPC Letters

**RSC:** J. Mat. Chem. A, Nanoscale, Chem. Comm, PhysChemChemPhys

**Elsevier:** Nano Energy, Surface Science, Electrochimica Acta

**Wiley:** Advanced Materials, Angewante Chemie, Advanced Functional Materials

### 3. Reviewer for International Funding Agencies:

- (i) European Research Council (ERC) Advanced Grants
- (ii) U.S. Dept. of Energy, Materials Science & Engineering Division (DOE-EPSCoR)
- (iii) Italian Ministry of Education, Universities and Research (MIUR)
- (iv) QNRF Grants– National Priorities Research Program (NPRP)

### 4. International Conference (As Main Organizer/Convener):

- I. Symposium D3, **EUROMAT, 2013**, Sevilla, Spain
- II. Symposium A, **EMRS Fall Meeting, 2014**, Warsaw, Poland
- III. ICCP-9, Singapore, **2015**
- IV. Symposium A, **EMRS Fall Meeting, 2015**, Warsaw, Poland
- V. Symposium L, **EMRS Fall Meeting, 2016**, Warsaw, Poland
- VI. PAN-IIT Webinar Series on Materials Simulation: A Virtual Guided Tour (2020)
- VII. CARE-2023, Harish-Chandra Research Institute(HRI)Prayagraj, 2<sup>nd</sup>-4<sup>th</sup> Feb, 2023

### Teaching Activity

#### A. Teaching Assignment in HRI Allahabad

- I. Quantum Mechanics -III
- II. Numerical Methods

#### B. Teaching Activity in IIT Indore:

- I. Statistical Physics (M.Sc. Theory Course since Fall, 2019)
- II. Atomic & Molecular Physics (M. Sc. Theory Course since Autumn, 2019)
- III. Numerical Methods and Computing (M.Sc. Theory Course Since Autumn, 2019)
- IV. Modern Physics (B. Tech Theory Course in Autumn, 2020)

Also, served as University Lecturer for Master degree courses in Pune University for 2007–2010: **I.** Advanced Numerical Analysis, **II.** Computational Methods in Physics.

### Research Thrusts and Endeavours

Materials Modeling for Energy Harvesting through cutting edge computational methodology is the prime focus of my research. The specific research interests are:

- ❖ Code Development for Solid-Liquid Interface and Transition Pathway Prediction
- ❖ Hybrid Perovskites & Ultra-thin 2D Materials for Solar Cells and LED.

- ❖ Solar Hydrogen and Thermal Fuel, Photocatalytic Water Splitting
- ❖ Catalytic Reaction Mechanism (HER, ORR & OER) on 2D Materials and Oxides.
- ❖ Efficient Cathode and Anode materials for Battery and Hybrid Supercapacitor
- ❖ Phonons based Stability (Dynamical) and Defect Formation Mechanism.
- ❖ Computational High-Pressure Physics: Structural and Phase Transformations

**In a Nutshell:** After completing my Ph.D on modeling semiconductor quantum dots for efficient solar cell materials, in collaboration between Bhabha Atomic Research Centre (BARC) and University of Pune, India, I moved to Max Planck Institute, Düsseldorf, Germany in **March, 2011** as a Max Planck Postdoctoral Fellow. I was involved in exploring different catalytic reaction mechanism based on electronic structure theory perspective. In **February, 2013**, I joined Materials Theory Division, Uppsala University, Sweden to work on photocatalytic Water Splitting, Efficient Battery Materials and Hybrid Perovskites Solar Cell. From **March, 2019**, I am leading Materials Theory for Energy Scavenging (MATES) Lab in Department of Physics, Indian Institute of Technology (IIT) Indore, as Assistant Professor. From **May, 2021**, I moved to India's premier theoretical research Institute, Harish-Chandra Research Institute (HRI), Allahabad as Reader and reestablished my research group there.

Presently, I have **170** International publications: **1**-Nature Materials (IF:41.2); **1**-Advanced Materials (IF:32.08); **1**-Materials Today (IF:26.94); **1**-Applied Catalysis B(IF:24.3); **4**-ACS Energy Letters (IF:23.99); **3**-Advanced Functional Materials (IF:19.92); **1**-Applied Physics Reviews (IF:19.51); **3**-Nano Energy (IF:19.07); **3**-ACS Nano (IF:18.03); **4**-Angewandte Chemie (IF:16.82); **2**-JACS (IF:16.38); **12**-Journal of Materials Chemistry A (IF:14.51); **2**-ACS Catalysis (IF:13.70); **2**-Small (IF:13.1); **2**-PNAS (IF:12.78); **6**-Chemistry of Materials(IF:10.51); **8**-ACS Applied Materials & Interfaces (IF:10.38); **1**-Chemical Science (IF:9.97); **1**-Advanced Optical Materials (IF:9.93); **1**-Journal of Power Sources (IF:9.79); **1**-ACS Sensors (IF:9.62); **1**-Solar RRL (IF:9.17); **2**-ChemSusChem (IF:9.14); **2**-Nanoscale (IF:8.31); **3**-Journal of Materials Chemistry C (IF:8.07); **2**-Applied Surface Science (IF:7.39); **3**-International Journal of Hydrogen Energy (IF:7.14); **8**-ACS Applied Energy Materials (IF:6.96); **5**-Journal of Physical Chemistry Letters (IF:6.89); **3**-Sustainable Energy Fuels (IF:6.81); **3**-APL

Materials (IF:6.63); **1**-Catalysis Today (IF:6.56); **2**-Catalysis Science & Technology (IF:6.18); **1**-Chemical Communication (IF:6.06); **1**-Solar Energy (IF:5.72); **1**-Nanoscale Advances (IF:5.59); **4**-Inorganic Chemistry (IF:5.44); **2**-Scientific Reports (IF:5.00); **3**-Dalton Transactions (IF:4.57); **9**-Journal of Physical Chemistry C (IF:4.18); **1**-Energy Technology (IF:4.15); **1**-ACS Omega (IF: 4.13); **3**-RSC Advances (IF:4.04); **4**-Applied Physics Letters (IF:3.97); **2**-Nanotechnology (IF:3.95); **7**-PhysChemChemPhys (IF:3.94)

[Total Citations > **5880**; h-index = **42**, Total Impact ~1450]. *High Impact (>6.0)*  
*Publications are denoted by \*\*\*\*\**

### **International Publications (170)**

1. \*\*\*\*\* Effect of Pre-Intercalation on Li-Ion Diffusion by Operando Investigation and Topochemical Single-Crystal Transformation, Y. Luo<sup>†</sup>, J. Handy<sup>†</sup>, Tisita Das<sup>†</sup>, J. Ponis<sup>†</sup>, R. Albers, Y-H Chiang, Matt Pharr, B. Schultz, L. Gobbato, D. C. Brown, **Sudip Chakraborty\***, Sarbajit Banerjee\*, **Nature Materials – Accepted (2024)**.
2. \*\*\*\*\* Establishing the Correlation between Rashba Spin Splitting and HER Activity Enhancement in Janus Structures, D. Kumar, **Sudip Chakraborty\*** **Journal of Material Chemistry A-Accepted (2024)**.
3. \*\*\*\*\* Zero-dimensional Tin Halide Perovskite with Anisotropic Photoconductivity and High Charge Carrier Lifetime for Selective Deep-UV Photodetection, A. Ajayakumar, C. Muthu, Manasa G. B., A. V. Dev, R. Nishikubo, **Sudip Chakraborty\***, A. Saeki, L. Dou, C. Vijayakumar\*, **Advanced Functional Materials, 34, 2304899 (2024)**.
4. \*\*\*\*\* Colloidal Aziridinium Lead Bromide Quantum Dots, Maryna I. Bodnarchuk, L. Feld, C. Zhu, S.C. Boehme, F. Bertolotti, J. Avaro, M. Aebli, S.H.Mir, N. Masciocchi, R. Erni, **Sudip Chakraborty**, A. Guagliardi, G. Raino, Maksym V. Kovalenko, **ACS Nano, 18, 5684 (2024)**
5. Unravelling Rashba effect through spin-texture evolution in uni-dimensional-confined halide-perovskite under compression, J. Kaur, **Sudip Chakraborty\***, **Physical Review Materials – Accepted (2024)**.

6. \*\*\*\*\* High-Performance One-Dimensional Halide Perovskite Crossbar Memristors and Synapses for Neuromorphic Computing, S. Vishwanath, B. Febriansyah, S. Ng, Tisita Das, J. Acharya, R. John, D. Sharma, P. Danajaya, M. Jagadeeswararo, N. Tiwari, M. Kulkarni, W. Lew, **Sudip Chakraborty\***, A. Basu, N. Mathews, **Materials Horizon - Accepted (2024)**.
7. \*\*\*\*\* Ultrasmall CsPbBr<sub>3</sub> Blue Emissive Perovskite Quantum Dots Using K-Alloyed Cs<sub>4</sub>PbBr<sub>6</sub> Nanocrystals as Precursors, C Otero-Martínez, M Zaffalon, Y Ivanov, N Livakas, L Goldoni, G Divitin, Sankalpa Bora, G. Saleh, F. Meinard, A. Fratelli, **Sudip Chakraborty**, L. Polavarapu, S. Brovelli, Liberato Manna, **ACS Energy Letters**, **9**, 2367(2024).
8. \*\*\*\*\* Sulfoxide-Functional Nanoarchitectonics of Mesoporous Sulfur-Doped C<sub>3</sub>N<sub>5</sub> for Photocatalytic Hydrogen Evolution, X. Guan, X Zhang, Z Li, S Deshpande, M Fawaz, N Dharmarajan, C Lin, Z. Lei, L. Hu, J-K. Huang, P. Kumar, Z. Sun, **Sudip Chakraborty**, A. Vinu, **Chemistry of Materials - Accepted(2024)**.
9. \*\*\*\*\* Incorporation of Bimetallic Sulfide with Carbon Nitride for Advanced Na-Ion Batteries, J. Lee, R. Bahadur, S.H. Mir, I. Bargoria, V. Perumalsamy, A. Ruban, X. Yu, M. Breese, J. Yi, **Sudip Chakraborty\***, A. Vinu, **Small**, **35**, 234587 (2024)
10. Tuning Optoelectronic Properties of K<sub>2</sub>TeBiO<sub>6</sub> through Cationic Interplay, Manasa G.B., **Sudip Chakraborty\***– **ACS Applied Optical Materials**, **2**, 254 (2024)
11. \*\*\*\*\* Ultra-Low Loaded Platinum Bonded Hexagonal Boron Nitride as Stable Electrocatalyst for Hydrogen Generation, R. Sadhukhan, A. Kumar, Ponnappa K.P., A. Guha, R. Arenal, **Sudip Chakraborty**, T. N. Narayanan, **ACS Applied Materials & Interfaces** , **16**, 8627 (2024).
12. \*\*\*\*\* CsPbCl<sub>3</sub>→CsPbI<sub>3</sub> Exchange in Perovskite Nanocrystals Proceeds Through a Jump-the-Gap Reaction Mechanism, Nikolaos Livakas, Stefano Toso, Yurii Ivanov, Tisita Das, **Sudip Chakraborty**, Giorgio Divitini, Liberato Manna, **JACS**, **145**, 20442 (2023).
13. \*\*\*\*\* Defects Tune the Strong Metal-Support Interactions in Copper Supported on Defected Titanium Dioxide Catalyst for CO<sub>2</sub> Reduction, R. Belgamwar, R. Verma,

Tisita Das, **Sudip Chakraborty**, P. Sarawade, V. Polshettiwar, **JACS**, **145**, **8634** (2023).

14. \*\*\*\*\* A Universal Strategy of Perovskite Ink-Substrate Interaction to Overcome the Poor Wettability of a Self-Assembled Monolayer for Reproducible Perovskite Solar Cells, A. Kulkarni, R. Sarkar, S. Akel, M. Haeser, B. Klingebiel, M. Wuttig, **Sudip Chakraborty\***, Michael Saliba\*, Thomas Kirchartz\*, **Advanced Functional Materials**, **2305812** (2023).
15. \*\*\*\*\* Improved Alcohol Oxidation through Combined Effects of Tensile Lattice Strain and Twin Defects in Core–Shell Electrocatalysts, T. Singha, S. Tomar, **Sudip Chakraborty**, S. Das, B. Satpati, **Small**, **2309736** (2024)
16. Pressure Driven Band Gap Narrowing in  $\text{Rb}_2\text{AgPdCl}_5$ : Towards Shockley–Queisser limit of Lead Free Double Perovskite, Showkat H. Mir, **Sudip Chakraborty\***, **Journal of Physical Chemistry C**, **127**, **19728** (2023).
17. Pressure Driven Optical Transitions in Non-toxic Double Perovskite with a Columnar-ordered B-Site Cation: Piezochromism without Phase Transformation, S. Mir, **Sudip Chakraborty\***, **Journal of Physical Chemistry C**, **127**, **14805** (2023).
18. Augmenting Bi-functional Catalytic Efficiency in Vanadium based Pseudomonolayer: Chemical Paradigm of Functionalization, Vacancy and External Stimuli, Dharendra Kumar, **Sudip Chakraborty\***, **International Journal of Hydrogen Energy**, **51**, **323** (2023).
19. Chalcogen Composition Driven Enhancement of Catalytic Efficiency in Zirconium based Monolayers: Insight from Reaction Coordinate Mapping, S. Tomar, **Sudip Chakraborty\***, **Sustainable Energy & Fuels**, **7**, **4668** (2023).
20. \*\*\*\*\* Unveiling and Understanding the Remarkable Enhancement in the Catalytic Activity by the Defect Creation in UIO-66 during the Catalytic Transfer Hydrodeoxygenation of Vanillin with Isopropanol, A. Kar, R. Sarkar, A. Manal, R. Kumar, **Sudip Chakraborty\***, R. Ahuja, R. Srivastava\*, **Applied Catalysis B**, **325**, **122385** (2023).



21. \*\*\*\*\* Efficient CO<sub>2</sub> utilization and sustainable energy conversion via aqueous Zn-CO<sub>2</sub> batteries, S. Kaur, M. Kumar, D. Gupta, Prajna P. Mohanty, Tisita Das, **Sudip Chakraborty**, R. Ahuja, T. Nagaiah, **Nano Energy**, **109**, 108242 (2023).
22. \*\*\*\*\* Combining  $\pi$ -Conjugation and Cation- $\pi$  Interaction for Water-2 Stable and Photoconductive One-Dimensional Hybrid Lead Bromide, T. Sheikh, G. Anilkumar, Tisita Das, A. Rahman, **Sudip Chakraborty\***, A. Nag\*, **Journal of Physical Chemistry Letters**, **114**, 1870 (2023).
23. \*\*\*\*\* Self-powered NH<sub>3</sub> synthesis by trifunctional Co<sub>2</sub>B based high power density Zn-air batteries, D. Gupta, A. Kafle, P. P. Mohanty, Tisita Das, **Sudip Chakraborty**, R. Ahuja, T. Nagaiah, **Journal of Materials Chemistry A**, **11**, 12223 (2023)
24. \*\*\*\*\* S-doped C<sub>3</sub>N<sub>5</sub> derived from thiadiazole for efficient photocatalytic hydrogen evolution, X.Guan, M.Fawaz, R.Sarkar, C.Lin, Z.Li,Z. Lei,N. Dharmarajan,P. Kumar, X. Zhang, J. Yang, L. Hu, T. Wu, **Sudip Chakraborty**, J. Yi, A. Vinu, **Journal of Materials Chemistry A**, **11**, 12837 (2023).
25. \*\*\*\*\* Pt nanoparticles sensitized vertical aligned large area MoS<sub>2</sub> flakes for enhanced and selective H<sub>2</sub> sensing at room temperature, R. Wadhwa, A. Kumar, R. Sarkar, P. P. Mohanty, D. Kumar, S. Deswal, P. Kumar, R. Ahuja, **Sudip Chakraborty**, M Kumar, **ACS Applied Nano Materials**, **6**, 2527 (2023).
26. Catching an Oxo Vanadate Porous Acetylacetonate Covalent Adaptive Catalytic Network that Renders Mustard-Gas Simulant Harmless, N. Das, R. Paul, S. Tomar, C. Biswas, **Sudip Chakraborty,\*** J. Mondal\*, **Inorganic Chemistry** (2024)
27. Conformational Disorder in a Hybrid 2D Perovskite with a Long Aliphatic Chain under Pressure, Y Lekina, D Bradley, Y Xiao, A Thanetchaiyakup, X Zhao, J Kaur, **Sudip Chakraborty**, H. S. Soo, J. Hanna, Shen, Ze Xiang, **Journal of Physical Chemistry C**, **127**, 16496 (2023).
28. Zinc Substituted Cobalt Phosphate [ZnCo<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>] as a Bifunctional Electrocatalyst, D. Singh, S. Singh, Ponnappa K. P., R. Rai, P. Chirawatkul, **Sudip Chakraborty**, M. Fichtner, P. Barpanda, **Inorganic Chemistry**, **62**, 12345 (2023).

29. Dual Vacancy Enriched Copper Sulfoselenide Superstructures: a Highly Promising HER Electrocatalyst in Acid, S. Kumaravel, Dharendra Kumar, S. Sankar, A. Karmakar, R. Madhu, K. Bera, H. Dhandapani, S. Nagappan, **Sudip Chakraborty\***, S. Kundu\*, **Catalysis Science & Technology**, **13**, 694 (2023).
30. \*\*\*\*\* Tuning Paradigm of External Stimuli Driven Electronic, Optical and Magnetic Properties in Hybrid Perovskites and Metal Organic Complexes, H. Banerjee, J. Kaur, M.K.Nazeeruddin\*, **Sudip Chakraborty\***, **Materials Today**, **60**, 183(2022).
31. \*\*\*\*\* Assessing the Drawbacks and Benefits of Ion migration in Lead Halide Perovskites, K. Sakhatskyi, R. John, A. Guerrero, S. Tsarev, S. Sabisch, Tisita Das, M. Gebhard, S. Yakunin, I. Cherniukh, M. Kotyrba, Y. Berezovska, M. Bodnarchuk, **Sudip Chakraborty**, Juan Bisquert, Maksym Kovalenko, **ACS Energy Letters**, **7**, 3401 (2022).
32. \*\*\*\*\*Morphology Tuned Pt<sub>3</sub>Ge Accelerates Water Dissociation to Industrial Standard Hydrogen Production over a wide pH Range, S. Mondal, S. Sarkar, D. Bagchi, Tisita Das, R. Das, A. Singh, Ponnappa K. P., C. Vinod, **Sudip Chakraborty**, S. Peter, **Advanced Materials**, **34**, 2202294 (2022).
33. \*\*\*\*\* Tuning Spin Texture and Spectroscopic Limited Maximum Efficiency through Chemical Composition Space in Double Halide Perovskites, J. Kaur, **Sudip Chakraborty\***, **ACS Applied Energy Materials**, **5**, 5579 (2022).
34. \*\*\*\*\* Rationalization of Double Perovskite Oxides as Energy Materials: A Theoretical Insight from Electronic and Optical Properties, Manasa G. B., **Sudip Chakraborty\***, **ACS Materials Au**, **2**, 655 (2022). [Invited Perspective for Rising Stars Special Issue]
35. \*\*\*\*\* High yield selective electrochemical conversion of N<sub>2</sub> to NH<sub>3</sub> via morphology-controlled silver phosphate under ambient conditions, D. Gupta, A. Kafle, S. Kaur, Prajna P. Mohanty, Tisita Das, **Sudip Chakraborty**, R. Ahuja, T. Nagaiah, **Journal of Materials Chemistry A**, **10**, 20616 (2022).

36. \*\*\*\*\* Single Atom Functionalization in Vanadium Dichalcogenide Monolayers: Towards Enhanced Electrocatalytic Activity, S. Tomar, P. Sen, **Sudip Chakraborty\***, **Sustainable Energy & Fuels**, **6**, 5337 (2022).
37. \*\*\*\*\* Complementary Effect of Functionalization, Vacancy Defects and Strain Engineering in activating the basal plane of monolayer FePS<sub>3</sub> for HER, Tisita Das, **Sudip Chakraborty**, P. Sen, **Sustainable Energy & Fuels**, **6**, 5621 (2022).
38. \*\*\*\*\* Diffusion mediated morphological transformation in bifunctional Mn<sub>2</sub>O<sub>3</sub>/CuO-(VO)<sub>3</sub>(PO<sub>4</sub>)<sub>2</sub>·6H<sub>2</sub>O for enhanced electrochemical water splitting, S. Bhowmick, A. Sarangi, C. Moi, **Sudip Chakraborty**, M. Qureshi, **ACS Applied Materials Interfaces**, **14**, 52204 (2022).
39. \*\*\*\*\* Incorporating Au<sub>11</sub> Nanocluster on MoS<sub>2</sub> Nanosheet Edges for Promoting Hydrogen Evolution Reaction at the Interface, S. Gratiou, A. Karmakar, D. Kumar, S. Kundu, **Sudip Chakraborty**, S. Mandal, **Nanoscale**, **14**, 7919 (2022).
40. \*\*\*\*\* Epitaxial growth of GaAs nanowires on synthetic mica by metal-organic chemical vapor deposition, A. Gopakumar, Ponnappa. K. P., X.Yuan, Z. Azimi, F. Kremer, Chennupati Jagadish, **Sudip Chakraborty\***, Hoe Tan\*, **ACS Applied Materials Interfaces**, **14**, 3395 (2022).
41. \*\*\*\*\* Probing Photoexcited Charge Carrier Trapping and Defect Formation in Synergistic Doping of SrTiO<sub>3</sub>, N. Koshi, D. Murthy, **Sudip Chakraborty**, S. C. Lee, S. Bhattacharjee, **ACS Applied Energy Materials**, **1**, 1159 (2022).
42. \*\*\*\*\* Theory abide experimental investigations on morphology driven enhancement of electrochemical energy storage performance for manganese titanate perovskites electrodes, N. Kitchamsetti, M. Samtham, P. Didwal, Dharendra Kumar, D. Singh, S. Bimli, P. Chikatea, D. Basha, S. Kumar, C. Park; **Sudip Chakraborty\***; R. Devan\*, **Journal Power Sources**, **538**, 231525(2022).
43. Nanocoral Architecture for Enhanced Hydrazine Assisted Water Oxidation: Insight from Experiment and Theory, N Sethulakshmi, S. Nellaiappan, Pinuppa K.P., Tisita

- Das, S. Irusta, **Sudip Chakraborty\***, S. Sharma\*, **Journal of Electroanalytical Chemistry**, **922**, 116776 (2022).
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141. \*\*\*\*\* Mapping Structural Changes in Electrode Materials: Application of the Hybrid eigenvector-following DFT Method to Layered  $\text{Li}_{0.5}\text{MnO}_2$ , Ieuan Seymour, **Sudip Chakraborty**, Derek Middlemiss, David J. Wales and Clare P. Grey, **Chemistry of Materials**, **27**, 5550 (2015).
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- 154.** A Possible Mechanism for the Emergence of Additional Band Gap due to Ti-O-C/Ti-C Bonds in TiO<sub>2</sub>-Graphene Hybrid System for Enhanced Photodegradation of Methylene Blue under Visible Light, S. Umrao, S. Abraham, F. Theil, S. Pandey, V. Ciobota, P. K. Shukla, C. Rupp, **Sudip Chakraborty**, R. Ahuja, J. Popp, B. Dietzek, A. Srivastava, **RSC Advances**, **4**, 59890 (2014).
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- 157.** Electronic density-of-states of amorphous vanadium pentoxide films: Electrochemical data and density functional theory calculations, I. Lykissa, Shu-Yi Li, M. Ramzan, **Sudip Chakraborty**, R. Ahuja, C. G. Granqvist and G. A. Niklasson, **Journal of Applied Physics**, **115**, 18, 183701 (2014).
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167. Oxygen impact on Quantum Confinement Effect for silicon clusters in different size regimes: ab-initio investigations, **Sudip Chakraborty\***, Ch. Rajesh, Shailaja Mahamuni, S. V. Ghaisas, **Eur. Phys. J D**, **64**, **2**, **331** (2011).
168. Quantum Confinement effect in pristine and oxygen covered silicon nanocrystals with surface states, **Sudip Chakraborty\***, Ch Rajesh, S. Mahamuni, S. V. Ghaisas, **J. Computational & Theoretical Nanoscience**, **8**, **9**, **1739** (2011).
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**Under Revision (5)**

1. Spin Texture Evolution of Rashba Splitting under Pressure: A Case Study of Inorganic Nitride Perovskite, Showkat Mir, **Sudip Chakraborty\***– **Under Revision.**
2. Emerging van der Waals Hetero-structures for Enhanced Photocatalytic Water Splitting Through Type-II Band Alignment, S. Tomar, **Sudip Chakraborty\*** – **Under Revision.**
3. Three-fold Impact on Reaction Coordinate Mapping of Zirconium based Trichalcogenide Pseudo-monolayers as Emerging Bi-functional Ultrathin Catalysts, Ponnappa K.P., **Sudip Chakraborty\*** – **Under Revision.**
4. Zirconium dichalcogenides based van der Waals Heterostructures for Efficient Schottky Barrier Solar Cells, L. Tatikondewar, **Sudip Chakraborty\***, **R. Ahuja, A. Kshirsagar** – **Under Revision**
5. Thermally-Induced Reversible Fluorochromism by Self-Trapped Excitonic Emission in a Two-Dimensional Hybrid Copper(I)-Halide Single Crystal, A. Dev, Manasa G.B., S. Deshpande, P. Mukherjee, A. Ajayakumar, C. Muthu, T. Okamoto, **Sudip Chakraborty\***, D. D. Sarma, V. Biju, C. Vijayakumar\* – **Under Revision.**

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**Invited Talks (Invited: 40)**

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- (i) Department of Chemistry, Cambridge University, 2<sup>nd</sup> July 2013.
- (ii) IWCCMP-2013, 27<sup>th</sup> September 2013.
- (iii) FIWAMEA -2014, Mekens, 8<sup>th</sup> May 2014.
- (iv) Angstrom Mini-Symposium, Uppsala University, 26<sup>th</sup> May 2015.
- (v) Materials Science & Engineering, NTU, Singapore, 4<sup>th</sup> August 2015.
- (vi) Energy Research Institute @ NTU (ERIAN), Singapore, 20<sup>th</sup> August 2015.
- (vii) IWCCMP-2015, 19<sup>th</sup> October 2015
- (viii) TCT Awarded Talk, MSE, NTU, Singapore, 18<sup>th</sup> July, 2016
- (ix) Energy Research Institute, NTU (ERIAN), Singapore, 22<sup>nd</sup> July, 2016
- (x) Symposium U (Halide Perovskites), ICMAT, MRS-Singapore, 22<sup>nd</sup> June, 2017
- (xi) Uppsala-Dalian Symposium Talk, 29<sup>th</sup> November, 2018
- (xii) Materials Research Society of India (MRSI), Kolkata, 12<sup>th</sup> February 2020.
- (xiii) Materials Simulation: A Virtual Guided Tour, PAN-IIT , May 21 -31, 2020.
- (xiv) International Webinar: Modern Aspects of Physics, MRC, August 13, 2020.
- (xv) Lecture in Faculty Development Program, MAKAUT, India, 16<sup>th</sup> Sep, 2020
- (xvi) International Webinar: RSCNN, HIT, India, 27<sup>th</sup> September, 2020
- (xvii) International Conference on Perovskites (nanoGe), 19<sup>th</sup> - 20<sup>th</sup> November, 2020
- (xviii) International Rhine Round Table (MRS Chapter Cologne) 4<sup>th</sup> December, 2020
- (xix) IPS-23, Lausanne, Switzerland, August 2-5, 2021
- (xx) Materials Research Society of India (MRSI), India, Dec 20-23, 2021.
- (xxi) Representing HRI CMP Research in HBNI-im-CMP, SINP, 23-24<sup>th</sup> June, 2022
- (xxii) QMAT 2022(Quantum Condensed Matter), IIT-K, 18<sup>th</sup>-22<sup>nd</sup> September, 2022.
- (xxiii) Resource Person for Refresher Course, Hyderabad University, 22<sup>nd</sup> Oct., 2022.
- (xxiv) YIMQCMT-2022, NISER, Bhubaneswar, 29<sup>th</sup> October - 1<sup>st</sup> November, 2022
- (xxv) Research Institute for Sustainable Energy (RISE), TCG-CREST, 1<sup>st</sup> Dec, 2022
- (xxvi) DCC- 2022, IACS, Kolkata, 2<sup>nd</sup>-3<sup>rd</sup> December, 2022
- (xxvii) International Workshop, CTFM, IIT Madras, 5<sup>th</sup>-6<sup>th</sup> December, 2022
- (xxviii) International School of CMSMEE, JNCASR Bangalore, 12-14 December, 2022.
- (xxix) DAE-SSPS Conference, 2022, 18<sup>th</sup> -22<sup>nd</sup> December, 2022
- (xxx) Indo-German International Conference (PDC-IT), IIT-M, 8<sup>th</sup> -11<sup>th</sup> March, 2023

- (**xxx**i) Indo-German International Conference (DEEPT-23),SRM,12<sup>th</sup> -15<sup>th</sup> March, 2023
- (**xxx**ii) Advances in Photovoltaic Materials and Devices (APMD 23), June 2-4, 2023
- (**xxx**iii) Emerging Materials, IISER Pune, India, July 13-15, 2023
- (**xxx**iv)Psi-K Namma Conference, JNCASR and IISc, Bangalore, July 24-28, 2023
- (**xxx**v) National Conference on Electronic Structure by IOP/TIFR, November 15-17,2023
- (**xxx**vi) Department of Chemistry, University of Cambridge, 12<sup>th</sup> December, 2023.
- (**xxx**vii) UK Catalysis Hub Conference, Oxfordshire, U.K. December, 18 -19, 2023
- (**xxx**viii)International Conference – ICFM -2024, IIT-Kharagpur, January 9-11, 2024
- (**xxx**ix) International Conference on Materials Genome, SRM, February 22-24, 2024
- (**x**l) iSNIOE<sup>2</sup> – 2024, Shiv Nadar Institute, Delhi NCR, March 20 - 23, 2024