

**Present Status**

Dr. Sudip Chakraborty (Ph.D in Physics)

Reader

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**DOB:** 15/05/1984

**Webpage:** - <http://www.sudiphys.wixsite.com/ceslab-sudip>




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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
- 2008 – 2011** : Senior Research Fellow, (Department of Atomic Energy Fellowship), Bhabha Atomic Research Centre (BARC) & University of Pune, India
- 2006 – 2008** : Junior Research Fellow, (Department of Atomic Energy 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 Calculation 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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- Ranked 2<sup>nd</sup> (UGC Master Degree Fellow) in All India Entrance, Pune University, **2004**
- Dr. Gokhale Scholarship, 1<sup>st</sup> year (top 3), M. Sc, University of Pune, **2005**.
- Junior (**2006**) Research Fellowship, Department of Atomic Energy, Govt. of India
- Senior (**2008**) Research Fellowship, Department of Atomic Energy, Govt. of India
- Max Planck Post Doctoral Fellowship, MPIE, Düsseldorf, Germany, **2011**.
- Carl-Tryggers Fellowship, Uppsala University, Sweden, **2013**.

- TCT Visiting Scientist Award, Singapore (40,000 SEK), 2016.

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### Project Grants

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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 as 1st Installment)

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### Scientific Activity and Organization

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1. **Scientific Editor:** Guest Editor for Special Issues in following journals:
  1. **Frontiers in Chemistry**
  2. **Catalysts**
  3. **European Physical Journal Special Topic (EPJST)**
2. **Scientific Reviewer:** JACS, ACS Nano, Chemistry of Materials; ACS Energy Letters.; J. Phys. Chem. Letters. J. Phys. Chem. C (ACS); Nanoscale; J. Mat. Chem. A; Chem. Comm.; PhysChemChemPhys (RSC); Surface Science; Electrochimica Acta; Nano Energy (Elsevier); International Journal of Quantum Chem. (Wiley)
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. **Scientific Talks (Invited - 27):**
  - (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) S. N. Bose National Centre for Basic Sciences, India, 10<sup>th</sup> December, 2015
- (ix) Saha Institute of Nuclear Physics (SINP), India, 31<sup>st</sup> December, 2015
- (x) Indian Association of Cultivation of Sciences (IACS), India, 7<sup>th</sup> Januray, 2016
- (xi) TCT Awarded Talk, MSE, NTU, Singapore, 18<sup>th</sup> July, 2016
- (xii) Energy Research Institute, NTU (ERIAN), Singapore, 22<sup>nd</sup> July, 2016
- (xiii) EMN Prague Meeting, Prague, 21<sup>st</sup> -24<sup>th</sup> June, 2016
- (xiv) Colloquium Talk, Harish-Chandra Research Institute (HRI), 2<sup>nd</sup> August, 2016
- (xv) Symposium U (Halide Perovskites), ICMAT, MRS-Singapore, 22<sup>nd</sup> June, 2017
- (xvi) Materials Engineering, Indian Institute of Science (IISc), India, 27<sup>th</sup> June 2017
- (xvii) Colloquium Talk, TIFR Hyderabad (TCIS), India, 30<sup>th</sup> January, 2018
- (xviii) Uppsala-Dalian Symposium Talk, 29<sup>th</sup> November, 2018
- (xix) Materials Research Society of India (MRSI), Kolkata, 12<sup>th</sup> February 2020.
- (xx) Materials Simulation: A Virtual Guided Tour, PAN-IIT , May 21 -31, 2020.
- (xxi) International Webinar: Modern Aspects of Physics, MRC, August 13, 2020.
- (xxii) Lecture in Faculty Development Program, MAKAUT, India, 16<sup>th</sup> Sep, 2020
- (xxiii) International Webinar: RSCNN, HIT, India, 27<sup>th</sup> September, 2020
- (xxiv) International Conference on Perovskites for Energy Harvesting: from  
Fundamentals to Devices (nanoGe), 19<sup>th</sup> - 20<sup>th</sup> November, 2020
- (xxv) International Rhine Round Table (hosted by the ACerS Chapter Germany and  
the MRS Chapter Cologne) 4<sup>th</sup> December, 2020
- (xxvi) International Conference on Photochemical Conversion & Storage of Solar  
Energy (IPS 23), Lausanne, Switzerland, August 2-5, 2021
- (xxvii) GSELOP-2021, Paris, France, August 23-25, 2021

#### 4. International Conference (Organizing Committee & Chairperson):

- (i) Symposium D3, **EUROMAT, 2013**, Sevilla, Spain (ii) Symposium A, **EMRS Fall Meeting, 2014**, Warsaw (iii) ICCP-9, Singapore, **2015** (iv) Symposium A, **EMRS Fall Meeting, 2015**, Warsaw (v) Symposium L, **EMRS Fall Meeting, 2016**, Warsaw. (vi) PAN-IIT Webinar Series on Materials Simulation: A Virtual Guided Tour (2020)

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### Research Supervision and Teaching Activity

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#### 1. After Joining Discipline of Physics, IIT Indore, India, March, 2019

##### A. Research Activity

I am leading my research group, Materials Theory for Energy Scavenging (MATES) Lab, in Physics, Indian Institute of Technology (IIT) Indore consisting of following:

- ❖ **6 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.
- ❖ **4 Masters** students (i) Mr. Jeevan Kumavat, (ii) Mr. Priyanka Yadav, (iii) Mr. Vardhman Diwadi, (iv) Mr. Diwakar Singh.

##### B. Teaching Activity

Teaching Assignment 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)
- III. Modern Physics (B.Tech Theory Course in Autumn, 2020)

#### 2. Before Joining Discipline of Physics, IIT Indore, India, March, 2019

##### A. Research Activity

- ❖ **4 Ph.D.** students, supervised by me officially, 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 Wårnå (10/2014 - 5/2019)
- ❖ **9 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)

**B. Teaching Activity**

Served as University Lecturer for Master degree courses in Department of Electronic Science, Pune University for 2007–2010: **I.** Advanced Numerical Analysis, **II.** Computational Methods in Physics **III.** Numerical Methods in Electronic Science.

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**Research Thrusts and Endeavours**

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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 (HER, ORR, OER) 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 **115** International publications: **2**-ACS Energy Letters(IF: 23.10); **1**-Advanced Functional Materials(IF: 18.81); **2**-Nano Energy(IF: 17.88); **2**-ACS Nano(IF: 15.88); **4**-Angewandte Chemie(IF: 15.34); **2**-ACS Catalysis(IF: 13.08); **7**-

Journal of Materials Chemistry A(IF: 12.73); **2**-PNAS(IF: 11.21); **1**-Adv. Optical Materials(IF: 9.93); **1**-Chemical Science(IF: 9.82); **5**-Chemistry of Materials(IF: 9.81); **5**-ACS Applied Materials & Interfaces(IF: 9.23); **2**-ChemSusChem(IF: 8.93); **1**-Solar RRL (IF:8.5);**1**-Nanoscale(IF:7.79);**1**-ACS Sensors(IF: 7.71); **3**-JMC-C(IF: 7.39); **1**-Catalysis Today(IF:6.77); **2**-Applied Surface Science(IF: 6.71); **5**-Journal of Physical Chemistry Letters(IF: 6.47); **1**-Chemical Communications(IF: 6.22); ; **1**-Ca.Sci.Tech(IF: 6.12); **6**-ACS Applied Energy Mater.(IF:6.02); **2**-IJHE(IF: 5.82); **1**-Inorg.Chem.(IF: 5.16); **2**-APL Materials (IF: 5.09) **1**-Nanoscale Adv(IF: 4.55); **2**-DaltonTrans(IF: 4.39); **2**-Scientific Reports(IF: 4.38); **6**-JPC-C(IF: 4.13); **3**-APL(IF: 3.79); **6**-PCCP(IF: 3.68); **5**-ChemPhysChem(IF: 3.1)

[Total Citations > 2720; h-index = 30, Total Impact ~ 760]. High Impact (>7.0)  
Publications are denoted by \*\*\*\*\*

### International Publications (115)

1. \*\*\*\*\* The Status Quo of Rashba Phenomena in Hybrid Perovskite Materials: Fundamentals and Implications, **Sudip Chakraborty\***, M. K. Nazeeruddin\*, **J. Phys. Chem. Letters**, **12**, 361 (2021)
2. \*\*\*\*\* Formation of Corrugated n=1 2D Tin-Iodide Perovskites and their Use as Lead-Free Solar Absorber, B. Febriansyah, Y. Lekina, J. Kaur, T. Hooper, P. Harikesh, T. Salim, M. Lim, T. Koh, **Sudip Chakraborty\***, Z. Shen, N. Mathews\*, J. England\* - **ACS Nano**, **15**, 6395 (2021).
3. \*\*\*\*\* An Organic-Inorganic Perovskitoid with Zwitterion Cysteamine Linker and Its Crystal-Crystal Transformation to Ruddlesden-Popper Phase, P. Kour, M. Reddy, S. Pal, S. Sidhik, T. Das, P. Pandey, S. Mukherjee\*, **Sudip Chakraborty\***, Aditya D. Mohite\*, S. B. Ogale, **Angewandte Chemie - Accepted(2021)**.
4. \*\*\*\*\* Halide Replacement with Complete Preservation of Crystal Lattice in Mixed-Anion Lanthanide Oxyhalides, M. Udayakantha, J. Handy, R. Davidson, J. Kaur, G. Villalpando, L. Zuin, **Sudip Chakraborty**, Sarbajit Banerjee, **Angewandte Chemie - Accepted (2021)**.

5. \*\*\*\*\* Unveiling the Roles of Lattice Strain and Descriptor Species on Pt-like Oxygen Reduction Activity in Pd-Bi catalysts, S. Sarkar, S. Ramarao, T. Das, R. Das, C. Vinod, **Sudip Chakraborty**, S Peter, **ACS Catalysis**, **11**, 800 (2021).
6. \*\*\*\*\* Lithium Silicates Nanosheets with Excellent Capture Capacity and Kinetics with Unprecedented Stability for High-Temperature CO<sub>2</sub> Capture, R. Belgamwar, A. Maity, T. Das, **Sudip Chakraborty**, C. Vinod, Vivek Polshettiwar, **Chemical Science**, **12**, 4825 (2021).
7. \*\*\*\*\* Concerted Ion-Migration and Diffusion Induced Degradation in Lead-Free Ag<sub>3</sub>BiI<sub>6</sub> Rudorffite Solar Cells under Ambient Conditions, A. Kulkarni, F. Ünlü, N. Pant, J. Kaur, C. Bohr, A. K. Jena, S. Öz, M. Yanagida, Y. Shirai, M. Ikegami, K. Miyano, Y. Tachibana, **Sudip Chakraborty**, Sanjay Mathur, Tsutomu Miyasaka, **Solar RRL – Accepted (2021)**
8. \*\*\*\*\* Structure-Tailored Non-Noble Metal-based Ternary Chalcogenide Nanocrystals for Pt-like Electrocatalytic Hydrogen Production, S Sarkar, A Rawat, Tisita Das, M Gaboardi, **Sudip Chakraborty**, C. Vinod, S. Peter, **ChemSusChem – Accepted (2021)**.
9. \*\*\*\*\* Self-Assembled Organic Cations Assisted Band-Edge Tailoring in Bismuth-based Perovskites for Enhanced Visible Light Absorption and Photoconductivity, J. K. Pious, Manasa G. B., C. Muthu, R. Nishikubo, A. Saeki, **Sudip Chakraborty\***, A. Takai, M. Takeuchi, C. Vijayakumar\*, **J. Phys. Chem. Letters**, **12**, 5758 (2021)
10. \*\*\*\*\* Stable Deep Blue Emission with Unity Quantum Yield in Organic-Inorganic Halide Perovskite 2D Nanosheets Doped with Cerium and Terbium at High Concentrations, S. Parveen, Ponnppa K. P., **Sudip Chakraborty\***, P. K. Giri\*, **Journal of Materials Chemistry C**, **9**, 2437(2021)
11. \*\*\*\*\* Organic-Inorganic Hybrid and Inorganic Halide Perovskites: Structural and Chemical Engineering, Interfaces and Optoelectronic Properties, S. Krishnamurthy, P. Pandey, J. Kaur, **Sudip Chakraborty\***, P. Nayak\*, A. Sadhanala\*, S. B. Ogale\*, **Journal of Physics D: Applied Physics**, **54**, 133002 (2021) [[Invited Topical Review](#)]

12. Charge Transfer Driven Interaction of CH<sub>4</sub>, CO<sub>2</sub> and NH<sub>3</sub> with TiS<sub>2</sub> monolayer: Influence of Vacancy Defect, T. Das, **Sudip Chakraborty\***, R. Ahuja, Y. Kawazoe, G. P. Das - **Catalysis Today**, **370**, 189 (2021).
13. Recent Progress in Al, K and Zn-ion Batteries: Experimental and Theoretical Viewpoints, D. Pal, Sudip Chakraborty\*, S. Chattopadhyay, **Energy Technology – Accepted (2021) (Invited Review Article)**
14. \*\*\*\*\* Bi<sup>3+</sup>- Er<sup>3+</sup> and Bi<sup>3+</sup>- Yb<sup>3+</sup> Co-doped Cs<sub>2</sub>AgInCl<sub>6</sub> Double Perovskite Near Infrared Emitter, H. Arfin, J. Kaur, **Sudip Chakraborty\***, A. Nag\*, **Angewandte Chemie**, **59**, 11307 (2020). (Selected as Hot Paper) [\[Featured Article\]](#)
15. \*\*\*\*\* Tweaking Nickel with Minimal Silver in a Heterogeneous Alloy of Decahedral Geometry to Deliver Platinum-like Hydrogen Evolution Activity, R. Majee, A. Kumar, T. Das, **Sudip Chakraborty**, S. Bhattacharyya, **Angewandte Chemie**, **59**, 2881 (2020).
16. \*\*\*\*\* ns<sup>2</sup> Electron (Bi<sup>3+</sup> and Sb<sup>3+</sup>) Doping in Lead-Free Metal Halide Perovskite Derivatives, H. Arfin†, A. Kshirsagar†, J. Kaur†, B. Mondal, Z. Xia, **Sudip Chakraborty\***, A. Nag\*, **Chemistry of Materials**, **32**, 10255 (2020).
17. \*\*\*\*\* Combinatorial design and computational screening of 2D transition metal tri-chalcogenide monolayers: Toward efficient catalysts for hydrogen evolution reaction, P. Sen, K. Alam, T. Das, R. Banerjee, **Sudip Chakraborty**, **J. Phys. Chem. Letters**, **11**, 3192 (2020).
18. \*\*\*\*\* Facets and Defects in Perovskites Nanocrystal for Photocatalytic CO<sub>2</sub> Reduction, S. Shyamal, S. Dutta, T. Das, **Sudip Chakraborty\***, Narayan Pradhan\*, **J. Phys. Chem. Letters**, **11**, 3608 (2020).
19. \*\*\*\*\* Solid State Synthesis of Stable and Color Tunable Cesium Lead Halide Perovskite Nanocrystals and Mechanism of High-Performance Photodetection in Monolayer MoS<sub>2</sub>/CsPbBr<sub>3</sub> Vertical Heterojunction, J. Ghosh, L. Mawlong, Manasa, G. B., M. Hossain, A. Pattison, W. Theis, **Sudip Chakraborty\***, P. K. Giri\*, **Journal of Materials Chemistry C**, **8**, 8917 (2020).
20. \*\*\*\*\* Shaping a Doped Perovskite Oxide with Measured Grain Boundary Defects to Catalyze Bifunctional Oxygen Activation for Rechargeable Zn-air Battery, R.

- Majee, T. Das, **Sudip Chakraborty**, S. Bhattacharyya - **ACS Applied Materials & Interfaces**, **12**, 40455 (2020).
21. \*\*\*\*\* Anisotropic photoconductivity and long-lived charge carriers in Bismuth-based one-dimensional perovskite with Typ-IIa Band Alignment, J. Pious, Manasa G.B., C. Muthu, N. Krishna, R. Nishikubo, A. Saeki, **Sudip Chakraborty\***, V. C. Nair\* - **Journal of Physical Chemistry Letters**, **11**, 6757 (2020).
22. \*\*\*\*\* Lewis acid-base interactions between polysulfides and boehmite enables stable room-temperature sodium–sulfur batteries, A. Ghosh, A. Kumar, T. Das, A. Ghosh, **Sudip Chakraborty**, M. Kar, D. R. MacFarlane, S. Mitra, **Advanced Functional Materials**, 2005669 (2020).
23. \*\*\*\*\* Emerging Piezochromism in Lead free Alkaline Earth Chalcogenide Perovskite  $AZrS_3$  ( $A = Mg, Ca, Sr$  and  $Ba$ ) under Pressure, A. Majumdar, A. Adeleke, **Sudip Chakraborty\***, R. Ahuja\*, **Journal of Materials Chemistry C**, **8**, 16392 (2020). [\[Featured Article – HOT Paper\]](#)
24. Understanding the interplay of stability and efficiency in A-site engineered lead halide perovskites, F. Ünlü, E. Jung, J. Haddad, A. Kulkarni, S. Öz, H. Choi, T. Fischer, **Sudip Chakraborty**, T. Kirchartz, S. Mathur, *Invited Perspective*, **APL Materials**, **8**, 070901 (2020). [\[Featured Article\]](#)
25. Emerging Piezochromism in Transparent Lead free Perovskite  $Rb_3X_2I_9$  ( $X = Sb, Bi$ ) under Compression: A Comparative Theoretical Insight, A. Majumdar, **Sudip Chakraborty\***, R. Ahuja, **Journal of Applied Physics**, **128**, 045102 (2020). [\[Featured Article\]](#)
26. Reaction Coordinate Mapping of Hydrogen Evolution Mechanism on  $Mg_3N_2$  Monolayer, A. Banerjee, **Sudip Chakraborty**, R. Ahuja, **International Journal of Hydrogen Energy**, **45**, 22848 (2020).
27. High exothermic dissociation in van-der-waals like hexagonal two dimensional nitrogene from first-principles molecular dynamics, A. Majumdar, X. Yang, W. Luo, S. Chowdhury, **Sudip Chakraborty**, R. Ahuja, **Applied Surface Science**, **529**, 146552 (2020).

28. Enhanced Electrocatalytic Activity in Geometrically Designed Epitaxial SrRuO<sub>3</sub> Thin Films, A. Biswas, G. S. Shanker, T. Das, R. Mandal, **Sudip Chakraborty\***, S. B. Ogale\*, **Applied Surface Science**, **529**, 147065 (2020).
29. \*\*\*\*\* Limiting Heterovalent B-site Doping in CsPbI<sub>3</sub> Nanocrystals: The Phase and Optical Stability, S. Bera, D. Ghosh, A. Dutta, S. Bhattacharyya, **Sudip Chakraborty\***, Narayan Pradhan\*, **ACS Energy Letters**, **4**, 1364 (2019).
30. \*\*\*\*\* Defect formations and pH-dependent kinetics in kröhnkite Na<sub>2</sub>Fe(SO<sub>4</sub>)<sub>2</sub>·2H<sub>2</sub>O based cathode for sodium-ion batteries: Resembling synthesis conditions through chemical potential landscape, T. Watcharatharapong, J. Thieprasert, **Sudip Chakraborty**, R. Ahuja, **Nano Energy**, **55**, 123 (2019).
31. \*\*\*\*\* A zero-dimensional lead-free hybrid perovskite with a quantum-well structure, J. Pious, A. Katre, C. Muthu, **Sudip Chakraborty**, S. Krishna, V. C. Nair, **Chemistry of Materials**, **31**, 3941 (2019).
32. \*\*\*\*\* Single atomic vacancy catalysis, J. Yang, Y. Wang, M. Lagos, S. Manichev, R. Fullon, X. Song, D. Voiry, **Sudip Chakraborty**, W. Zhang, P. Batson, L. Feldman, T. Gustafsson, Manish Chhowalla, **ACS Nano**, **13**, 9958 (2019).
33. \*\*\*\*\* Rashba-Triggered Electronic and Optical Properties Tuning in Mixed Halide Hybrid Perovskites, A. Banerjee, **Sudip Chakraborty\***, R. Ahuja, **ACS Applied Energy Materials**, **2**, 6990 (2019).
34. \*\*\*\*\* Emergence of Si<sub>2</sub>BN monolayer as Efficient HER catalyst under co-functionalization influence, D. Singh, **Sudip Chakraborty\***, R. Ahuja, **ACS Applied Energy Materials**, **2**, 8441 (2019).
35. \*\*\*\*\* Functionalization and Defect Driven HER and OER Mechanism on Quasi 2D TiO<sub>2</sub> HNS, T. Das, **Sudip Chakraborty\***, G. P. Das, R. Ahuja, **ACS Applied Energy Materials**, **2**, 5074 (2019).
36. \*\*\*\*\* Sodium intercalation mechanism, structure evolutions and electrochemical properties in non-stoichiometric alluaudite-type sodium iron sulfate T. Watcharatharapong, **Sudip Chakraborty\***, R. Ahuja, **Journal of Materials Chemistry A**, **7**, 17446 (2019).

37. \*\*\*\*\* Defect Thermodynamics in Non-stoichiometric Alluaudite based Polyanionic Materials for Na-ion Batteries, T. Watcharatharapong, **Sudip Chakraborty\***, R. Ahuja, **ACS Applied Materials & Interfaces**, **11**, 32856 (2019).
38. \*\*\*\*\* Designing a new family of oxonium-cation based structurally diverse organic-inorganic hybrid iodoantimonate crystals, S. Parmar, S. Pal, A. Biswas, S. Gosavi, **Sudip Chakraborty\***, S. Ogale, **Chemical Communications**, **55**, 7562 (2019).
39. Composition Dependent Tuning of Electronic and Magnetic Properties in Transition Metal Substituted Rock-Salt MgO, K. Klaa, S. Labidi, A. Banerjee, **Sudip Chakraborty**, M. Labidi, A. Amara, M. Bououdina, R. Ahuja, **J. Magn. Magn. Mater**, **475**, 44 (2019).
40. Cesium Bismuth Iodide Solar Cells from Systematic Molar Ratio variation of CsI and BiI<sub>3</sub>, M. Johansson, B. Philippe, A. Banerjee, D. Phuyal, S. Mukherjee, **Sudip Chakraborty**, M. Cameau, H. Zhu, R. Ahuja, G. Boschloo, H. Rensmo, E. Johansson, **Inorganic Chemistry**, **58**, 12040 (2019).
41. Cu-doped nickel oxide interface layer with nanoscale thickness for efficient and highly stable printable carbon-based perovskite solar cell, A. Bashir, L. Haur, S. Shukla, D. Gupta, T. Baikie, **Sudip Chakraborty**, R. Patidar, A. Bruno, Subodh Mhaisalkar, Z. Akhter, **Solar Energy**, **182**, 225 (2019).
42. Phase evolution in calcium molybdate nanoparticles as a function of synthesis temperature and its electrochemical effect on energy storage, M. Minakshi, D. Mitchell, C. Baur, J. Chable, A. Barlow, M. Fichtner, A. Banerjee, **Sudip Chakraborty**, R. Ahuja, **Nanoscale Advances**, **1**, 565 (2019). [[Most Popular Articles Collection of Nanoscale Advances](#)]
43. TiS<sub>2</sub> Monolayer Emerging as Ultrathin Bifunctional Catalyst: Influence of Defect and Functionalization, T. Das, **Sudip Chakraborty\***, R. Ahuja, G. P. Das, **ChemPhysChem**, **20**, 4 (2019).
44. \*\*\*\*\* In Pursuit of Bifunctional Catalytic Activity in PdS<sub>2</sub> pseudo-monolayer through Reaction Coordinate Mapping, D. Saraf, **Sudip Chakraborty\***, A. Kshirsagar, R. Ahuja, **Nano Energy**, **49**, 283 (2018).

45. \*\*\*\*\* Mechanistic Insight of Enhanced Hydrogen Evolution Reaction Activity of Ultra-thin h-BN Modified Pt Electrodes, A. Guha, T. Vineesh, A. Sekar, S. Narayanaru, M. Sahoo, S. Nayak, **Sudip Chakraborty\***, T. Narayanan, **ACS Catalysis**, **8**, 6636 (2018).
46. \*\*\*\*\* Simultaneous enhancement in charge separation and onset potential for water oxidation in BiVO<sub>4</sub> photoanode by W-Ti codoping, X. Zhao, J. Hu, B. Wu, A. Banerjee, **Sudip Chakraborty \***, J. Feng, Z. Xhao, S. Chen, R. Ahuja, T. C. Sum, Z. Chen, **J. Mater. Chem. A**, **6**, 16965 (2018).
47. \*\*\*\*\* Molecular and self-trapped excitonic contributions to the broadband luminescence in diamine based low dimensional hybrid perovskite systems, S. Krishnamurthy, R. Naphade, W. Mir, S. Gosavi, **Sudip Chakraborty\***, R. Vaidhyanathan, S. Ogale, **Advanced Optical Materials**, **17**, 1800751 (2018).
48. \*\*\*\*\* Investigation on Organic Molecule Additive for Moisture Stability and Defect Passivation via Physisorption in CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> based Perovskite, S. Singh, B. Sharma, S. B. Gangadhar, A. Dey, **Sudip Chakraborty**, K. L. Narashimhan, P. Bhargava, Dinesh Kabra, **ACS Applied Energy Mater.** **1**, 1870 (2018).
49. \*\*\*\*\* Maneuvering the Physical Properties and Spin States to Enhance the Activity of La-Sr-Co-Fe-O Perovskite Oxide Nanoparticles in Electrochemical Water Oxidation, R. Majee, **Sudip Chakraborty**, H. Salunke, Sayan Bhattacharaya, **ACS Applied Energy Mater.** **1**, 3342 (2018).
50. \*\*\*\*\* Scrupulous Probing of Bifunctional Catalytic Activity of Borophene Monolayer: Mapping Reaction Coordinate with Charge Transfer, A. Banerjee, **Sudip Chakraborty\***, N. Jena, R. Ahuja, **ACS Applied Energy Mater.** **1**, 3578 (2018).
51. Current Computational Trends in Polyanionic Cathode Materials for Li and Na batteries, **Sudip Chakraborty\***, A. Banerjee, T. Watcharatharapong, R. Araujo, R. Ahuja, **J. Phys: Condensed Matter**, **30**, 283003 (2018). [\[Invited Topical Review\]](#)
52. Synthesis and Optical Properties of Colloidal M<sub>3</sub>Bi<sub>2</sub>I<sub>9</sub> (M = Cs, Rb) Perovskite Nanocrystals, J. Pal, A. Bhunia, **Sudip Chakraborty**, S. Manna, S. Das, A. Diwan, S. Datta, A. Nag, **J. Phys. Chem. C**, **122**, 10643 (2018).
53. Defected and Functionalized Germanene based Nanosensors under Sulfur Comprising

- Gas Exposure, T. Hussain, T. Kaewmaraya, **Sudip Chakraborty\***, H. Vovusha, V. Amornkitbamrung, R. Ahuja, **ACS Sensors**, **3**, 867 (2018).
54. New Concept on Photocatalytic Degradation of Thiophene Derivatives: Experimental and DFT studies, N. Djouambi, C. Bougheloum, A. Messalhi, M. Bououdina, A. Banerjee, **Sudip Chakraborty**, R. Ahuja, **J. Phys. Chem. C**, **122**, 15646 (2018).
55. A combined theoretical and experimental approach of a new ternary metal oxide in molybdate composite for hybrid energy storage capacitors, M. Minakshi, W. Teeraphat, **Sudip Chakraborty**, R. Ahuja, **APL Materials** **6**, 047701 (2018).
56. Cystamine-configured lead halide based 2D hybrid molecular crystals: Synthesis and photoluminescence systematics, S. Krishnamurthy, P. Kour, A. Katre, S. Gosavi, **Sudip Chakraborty\***, S. Ogale, **APL Materials**. **6**, 114204 (2018).
57. Theoretical Investigation of Bifunctional Catalytic Activity of  $\text{Al}_2\text{C}$  for Hydrogen and Oxygen Evolution Reaction, R. Almeida, A. Banerjee, **Sudip Chakraborty\***, J. Almeida, R. Ahuja, **ChemPhysChem**, **19**, 141 (2018).
58. Saline Accelerates Oxime Reaction with Aldehyde and Keto Substrates at Physiological pH, S. Wang, G. Nawale, S. Kadekar, O. Oommen, N. Jena, **Sudip Chakraborty**, J. Hilborn, O. P. Varghese, **Sci. Rep.**, **8**, 2193 (2018).
59. \*\*\*\*\* Rational Design: A High-Throughput Computational Screening and Experimental Validation Methodology for Lead-free and Emergent Hybrid Perovskites, **Sudip Chakraborty\***, W. Xie, N. Mathews, M. Sherburne, R. Ahuja, Mark Asta, S. G. Mhaisalkar, **ACS Energy Letters**, **2**, 837 (2017).
60. \*\*\*\*\* Bromination Induced Stability Enhancement with Multivalley Optical Response Signature in Guanidinium  $[\text{C}(\text{NH}_2)_3]^+$  Based Hybrid Perovskite Solar Cells, A. Banerjee, **Sudip Chakraborty\***, R. Ahuja, **J. Mater. Chem. A**, **5**, 18561 (2017).
61. \*\*\*\*\* Mechanistic Study of Na-ion diffusion and small hole polaron formation in  $\text{Na}_2\text{Fe}(\text{SO}_4)_2 \cdot 2\text{H}_2\text{O}$  cathode material for battery applications, T. Watcharatharapong, J. Thieprasert, P. Barpanda, R. Ahuja, **Sudip Chakraborty\***, **J. Mater. Chem. A**, **5**, 21726 (2017).
62. \*\*\*\*\* Effect of transition metal cations on stability enhancement for molybdate based hybrid supercapacitor, T. Watcharatharapong, M. Minakshi, **Sudip**

- Chakraborty\***, D. Li, G. Shafiullah, R. Aughterson, R. Ahuja, **ACS Applied Materials & Interfaces**, **9**, 17977 (2017).
63. \*\*\*\*\* Black phosphorus as efficient metal-free photocatalyst for hydrogen evolution, S. Muduli, V. Eswaraiah, X. You, S. Kulkarni, A. Katre, **Sudip Chakraborty**, S. Chen, T. Sum, X. Rong, N. Mathews, **J. Mater. Chem. A**, **5**, 24874 (2017).
64. A Comparative Study of Hydrogen Evolution Reaction on WS<sub>2</sub> and PtS<sub>2</sub> pseudo-monolayer: Insight based on Density Functional Theory, S. H. Mir, **Sudip Chakraborty\***, J. Warna, S. Narayan, P. C. Jha, P. K. Jha, R. Ahuja, **Catalysis Science & Technology**, **7**, 687 (2017).
65. Role of relativity in high-pressure phase transitions in thallium, K. Kotmool, **Sudip Chakraborty**, T. Bovornratanaraks, R. Ahuja, **Scientific Reports**, **7**, 42983 (2017).
66. Poor Photovoltaic Performance of Cs<sub>3</sub>Bi<sub>2</sub>I<sub>9</sub>: An Insight through First Principles Calculations, B. Ghosh, **Sudip Chakraborty**, C. Guet, H. Wei, S. Li, S. G. Mhaisalkar, N. Mathews, **J. Phys. Chem. C**, **121**, 17062 (2017).
67. Valence Level Character in a Mixed Perovskite Material and Determination of the Valence Band Maximum from Photoelectron Spectroscopy: Variation with Photon Energy, B. Philippe, T. Jacobsson, J. Correa-Baena, N. Jena, A. Banerjee, **Sudip Chakraborty**, U. Cappel, R. Ahuja, A. Hagfeldt, M. Odelius, H. Rensmo, **J. Phys. Chem. C**, **121**, 26655 (2017).
68. Na<sub>2.54</sub>Co<sub>1.73</sub>(SO<sub>4</sub>)<sub>3</sub> as a New Member of *Alluaudite* Family of High-Voltage Sodium Battery Cathode, D. Dwibedi, R. Gond, A. Dayamani, R. Araujo, **Sudip Chakraborty**, R. Ahuja, P. Barpanda, **Dalton Transactions**, **46**, 55 (2017).
69. Cluster assembly route to a novel octagonal two-dimensional ZnO monolayer, P. Gaikwad, P. Pujari, **Sudip Chakraborty**, A. Kshirsagar, **J. Phys. Condensed Matter**, **29**, 335501 (2017).
70. Improved Sensing Characteristics of Methane on ZnO Nano Sheets Upon Implanting Defects and Foreign Atoms Substitution, T. Hussain, T. Kaewmaraya, M. Khan, **Sudip Chakraborty\***, M. Islam, V. Amornkitbamrung, R. Ahuja, **Nanotechnology**, **28**, 415502 (2017).

71. Design and Control of Cooperativity in Spin-Crossover in Metal-organic Complexes: A Theoretical Overview, H. Banerjee, **Sudip Chakraborty**, T. Saha Dasgupta, **Inorganics**, **5**, 47 (2017). [\[Invited Review Article\]](#)
72. \*\*\*\*\* High pressure induced distortion in Face-centered-cubic phase of Thallium, K. Kotmool, B. Li, **Sudip Chakraborty**, T. Bovornratanaraks, W. Luo, Ho-Kwang Mao, R. Ahuja, **PNAS**, **113**, 11143 (2016).
73. \*\*\*\*\* Predicting Electrochemical Properties and Ionic Diffusion in  $\text{Na}_{2+2x}\text{Mn}_{2-x}(\text{SO}_4)_3$ : Crafting a Promising High Voltage Cathode Material, R. Araujo, M. Islam, **Sudip Chakraborty\***, R. Ahuja, **J. Mater. Chem. A**, **4**, 451 (2016) (Selected as Journal HOT article).
74. \*\*\*\*\* Rationalizing Hydrogen and Oxygen Evolution Reaction Activity of Two-dimensional Hydrogenated Silicene and Germanene, C. Rupp, **Sudip Chakraborty\***, J. Anversa, R. Baierle, R. Ahuja, **ACS Appl. Mater. Interfaces**, **8**, 1536 (2016).
75. \*\*\*\*\* Cationic Effect on Pressure driven Spin-State Transition and cooperativity in Hybrid Perovskites, Hrishit Banerjee, **Sudip Chakraborty**, T. Saha-Dasgupta, **Chemistry of Materials**, **28**, 8379 (2016).
76. \*\*\*\*\* Synthesis, structural and electrochemical properties of sodium nickel phosphate for energy storage devices, M. Minakshi, D. Mitchell, R. Jones, W. Teeraphat, **Sudip Chakraborty**, R. Ahuja, **Nanoscale**, **8**, 11298 (2016).
77. \*\*\*\*\* Ionothermal Synthesis of High-voltage *Alluaudite*  $\text{Na}_2\text{Fe}_2(\text{SO}_4)_3$  Sodium Insertion Compound: Structural, Electronic and Magnetic Insight, D. Dwibedi, C. D. Ling, R. Araujo, **Sudip Chakraborty**, S. Duraisamy, N. Munichandraiah, R. Ahuja, P. Barpanda, **ACS Appl. Mater. Interfaces**, **6**, 6982 (2016).
78. Probing the Anisotropic Ion Diffusion in 2-D in Lithium Titanium Niobate Anode for Li-ion Battery, S. Das, D. Dutta, R. Araujo, **Sudip Chakraborty**, R. Ahuja, A. J. Bhattacharyya, **PhysChemChemPhys**, **18**, 22323 (2016).
79. First principle investigation of  $\text{Na}_2\text{M}_2(\text{SO}_4)_3$  (M=Fe, Mn, Co and Ni): Towards High Voltage Sodium Battery Applications, R. Araujo, **Sudip Chakraborty\***, P. Barpanda, R. Ahuja, **PhysChemChemPhys**, **18**, 9658 (2016).

80. High pressure driven superconducting critical temperature tuning in  $\text{Sb}_2\text{Se}_3$  topological insulator, J. Anversa, **Sudip Chakraborty\***, P. Piquini, R. Ahuja, **Applied Physics Letters**, **108**, 212601 (2016).
81. Time Dependent DFT Investigation of Optical Response in Pristine and Gd Doped  $\text{Al}_2\text{O}_3$ , S. Kumavat, **Sudip Chakraborty\***, A. B. Rahane, M. D. Deshpande, R. Ahuja, **RSC Advances**, **6**, 72537 (2016).
82. Two-dimensional Boron: Lightest Catalyst for Hydrogen and Oxygen Evolution Reaction, S. Mir, **Sudip Chakraborty\***, P. K. Jha, J. Warna, H. Soni, P. Jha, R. Ahuja, **Applied Physics Letters**, **109**, 053903 (2016).
83. Nanostructured materials for solid-state hydrogen storage: a review of the achievement of COST Action MP1103, E. Callini, K. A-Zinsou, R. Ahuja, J. Ares, S. Bals, N. Biliskov, **Sudip Chakraborty et al. Int. J. Hydrogen Energy**, **41**, 14404 (2016). [\[Invited Review Article\]](#)
84. Rare earth functionalization effect in optical response of ZnO nano clusters, M. Mahabal, M. Deshpande, **Sudip Chakraborty**, T. W. Kang, R. Ahuja, **Eur. Phys. J D**, **73**, 1 (2016).
85. Defect and Substitution Induced Silicene Sensor to Probe Toxic Gases, T. Hussain, T. Kaewamaraya, **Sudip Chakraborty\***, R. Ahuja, **Journal of Physical Chemistry C** **120**, 25256 (2016).
86. \*\*\*\*\* 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).
87. \*\*\*\*\* Defect Engineered  $\text{g-C}_3\text{N}_4$  for Efficient Visible Light Photocatalytic Hydrogen Production, Q. Tay, P. Kanhere, C. Ng, S. Chen, **Sudip Chakraborty**, A. Huan, T. Sum, R. Ahuja, Z. Chen, **Chemistry of Materials**, **27**, 4930 (2015).
88. \*\*\*\*\*  $\text{Na}_{2.44}\text{Mn}_{1.79}(\text{SO}_4)_3$ : A new member of alluaudite family of insertion compound for sodium ion batteries, D. Dwibedi, R. Araujo, **Sudip Chakraborty**, P. Shanbogh, N. Sundaram, R. Ahuja, P. Barpanda, **J. Mater. Chem. A**, **3**, 18564 (2015).
89. \*\*\*\*\* Hydrogen storage materials for mobile and stationary applications: Current

- state of the art, Q. Lai, A. Thornton, M. Hill, Z. Haung, H.K. Lui, Z. Guo, M. Paskevicius, D. Sheppard, C. Buckley, A. Banerjee, **Sudip Chakraborty**, R. Ahuja, K.F. Aguey-Zinsou, **ChemSusChem**, **8**, 2789 (2015). [\[Invited Review Article\]](#)
90. The effect of impurities in ultra-thin hydrogenated silicene and germanene: A first principles study, C. Rupp, **Sudip Chakraborty**, R. Ahuja, R. Baierle, **PhysChemChemPhys**, **17**, 22210 (2015).
91. Unveiling the charge migration mechanism in Na<sub>2</sub>O<sub>2</sub>: Implications to sodium air batteries, Rafael B. Araujo, **Sudip Chakraborty\***, R. Ahuja, **PhysChemChemPhys**, **17**, 8203 (2015).
92. Substitution induced band structure shape tuning in hybrid perovskites (CH<sub>3</sub>NH<sub>3</sub>Pb<sub>1-x</sub>Sn<sub>x</sub>I<sub>3</sub>) for efficient solar cell applications, P. Kanhere, **Sudip Chakraborty\***, C. Rupp, R. Ahuja, Z. Chen, **RSC Advances**, **5**, 107497 (2015).
93. Synthesis, crystal and electronic structure of sodium metal phosphate for hybrid capacitor in non-aqueous electrolyte, M. S. Manickam, W. Teeraphat, **Sudip Chakraborty**, R. Ahuja, S. Duraisamy, P. T. Rao, N. Munichandraiah, **Dalton Transactions**, **44**, 20108 (2015).
94. Highly Sensitive and Selective Gas Detection Based on Silicene, J. Prasongkit, R. G. Amorim, **Sudip Chakraborty**, R. Ahuja, R. H. Scheicher, V. Amornkitbamrung, **J. Phys. Chem. C**, **119**, 16934 (2015).
95. Improvement in Hydrogen Desorption from  $\beta$  and  $\gamma$ -MgH<sub>2</sub> upon Transition Metal Doping, T. Hussain, T. A. Maark, **Sudip Chakraborty**, R. Ahuja, **ChemPhysChem**, **16**, 12, 2557 (2015). (Selected as VIP and Cover Article)
96. The Effect of Morphology and Confinement on the High-Pressure Phase Transition in ZnO Nanostructure, K. Kotmool, T. Bovornratanaraks, **Sudip Chakraborty**, R. Ahuja, **Journal of Applied Physics**, **117**, 114309 (2015).
97. BC<sub>3</sub> Sheet Functionalized with Lithium Rich Species Emerging as a Reversible Hydrogen Storage Material, T. Hussain, **Sudip Chakraborty\***, T. W. Kang, B. Johansson, R. Ahuja, **ChemPhysChem**, **16**, 634 (2015).
98. \*\*\*\*\* Revealing an unusual transparent phase of superhard Iron Tetraboride under high pressure, K. Kotmool, T. Kaewmaraya, **Sudip Chakraborty**, J. Anversa, T.

- Bovornratanaraks, W. Luo, H. Gou, P.C. Piquini, T. W. Kang, Ho-kwang Mao, R. Ahuja, **PNAS** **111**, 17050 (2014)
99. 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).
100. Enhancement of energy storage capacity of Mg functionalized silicene and silicane under external strain, T. Hussain, **Sudip Chakraborty**, A. De Sarkar, B. Johansson, Rajeev Ahuja, **Applied Physics Letters**, **105**, 125903 (2014).
101. Mono-and co-doped NaTaO<sub>3</sub> for visible light photocatalysis, P. Kanhere, P. Shenai, **Sudip Chakraborty**, R. Ahuja, J. Zheng, Z. Chen, **PhysChemChemPhys**, **16**, 30, 16085 (2014).
102. 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).
103. Stabilizing a hexagonal Ru<sub>2</sub>C via Lifshitz transition under pressure, W. Sun, **Sudip Chakraborty\***, R. Ahuja, **Applied Physics Letters**, **103**, 251901 (2013).
104. Functionalization of hydrogenated silicene with alkali and alkaline earth metals for efficient hydrogen storage, T. Hussain, T. Kaewmaraya, **Sudip Chakraborty\***, R. Ahuja, **PhysChemChemPhys**, **15**, 43, 18900 (2013).
105. Metal-Functionalized Silicene for Efficient Hydrogen Storage, T. Hussain, **Sudip Chakraborty\***, R. Ahuja, **ChemPhysChem**, **14**, 15, 3463 (2013).
106. Electronic and optical properties of agglomerated hydrogen terminated silicon nanoparticles, P. Francis, S. Patil, Ch. Rajesh, **Sudip Chakraborty**, S. Mahamuni, C. V Dharmadhikari, S. V. Ghaisas, **Eur. Phys. J D**, **67**, 144 (2013).
107. Relative Localization Prediction in Covalent Clusters: an ab-initio Theory Driven Quest, **Sudip Chakraborty\***, S. V. Ghaisas, **Adv. Sci. Lett.** **18**, 5, 208 (2012).
108. Optical Properties Of Gallium Oxide Clusters From First-Principles Calculations, Amol B. Rahane, M. D. Deshpande, **Sudip Chakraborty**, **J. Phys. Chem. A**

- 116, 43, 10559 (2012).
109. First principles based adsorption comparison of Group-IV elements (C, Si, Ge, Sn) on Au/Ag (111) surface, **Sudip Chakraborty\***, Ch. Rajesh, **J. Nanopart. Research** **14**, **10**, 1187 (2012).
110. An ab-initio study of silicon adsorption on metallic surfaces (Au/Ag): Novel perspective to explore chemical bonding, **Sudip Chakraborty\***, S. V. Ghaisas, Chiranjib Majumder, **Eur. Phys. J B**, **85**, **7**, 227 (2012).
111. Structural and Optical Properties of Oxygenated Silicon Quantum Dots, **Sudip Chakraborty\***, C. Rajesh, S. Mahamuni, S. Ghaisas, **Adv. Sci. Lett.** **4**, 3580 (2011).
112. 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).
113. 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).
114. Structure and Energetics of Silicon clusters adsorbed on Au (111) Surface: first principles study, **Sudip Chakraborty**, S. V. Ghaisas and Chiranjib Majumder, **International Journal of Nanotechnology**, **7**, **9**, 833 (2010).
115. Ab-initio Calculation for the Study of Nano Scale Silicon-based Structure, **Sudip Chakraborty\***, G. Shashidhar, S. V. Ghaisas, V. Sundararajan, **Solid State Phenomena**, **139**, 113 (2008).