Curriculum Vitae

Name: **DR. PRANAB SARKAR**

Date of Birth: **12.06.1969**

Marital Status: **Married**

Nationality: **Indian**

Current Designation: **Professor in Chemistry**

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(a) Official: **Dept. of Chemistry, Visva-Bharati (Central University), Santiniketan – 731235, India**
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Field of Specialization:
Computational Materials Science: Development and Implementation of SCC-DFTB parameters for Large Scale Computations, Solar Cell Materials, Non-Adiabatic Molecular Dynamics Simulations (NAMD), 2D Nanomaterials, Spintronics and Energy Storage Materials, Homogeneous and Heterogeneous Catalysis, Metal/Covalent Organic Frameworks, High Entropy Materials for catalysis

Academic career and professional attainments:

(a) Degree	Institution	Year	Remarks
B.Sc. (Hons. in Chemistry)	**The University of Burdwan**	**1989**	
M.Sc. (Chemistry)	**The University of Burdwan**	**1991**	
Ph. D.	**IACS (Jadavpur University)**	**1997**	

(b) Positions Held	Institution	From	To
Postdoctoral Researcher	**University of Montreal, Canada**	**1997**	**1998**
Visiting Scientist	**University of Saarlandes, Germany**	**2001**	**2003**
Assistant Professor	**Visva-Bharati (Central University)**	**1998**	**2007**
Associate Professor	**Visva-Bharati (Central University)**	**2007**	**2010**
Professor	**Visva-Bharati (Central University)**	**2010**	**Present**

(c) Awards / Special Attainments

i. **University Gold medal and Burdwan Sammilani Gold medal for securing the first position in M.Sc. Examination**
ii. **CSIR research fellowship award, Govt. of India**
iii. **CRSI Bronze Medal, Chemical Research Society of India, 2019**
iv. **UGC Mid-Career Awards, 2020**
v. **Indian National Science Academy (INSA) Teachers Award, 2021**
vi. **Fellow of West Bengal Academy of Science and Technology, 2022**

Number of Publication:

(a) International Journal: **205**
(b) National Journal: **5**
(c) Book/Book Chapter**: 7**

Number of Ph.D Students:

(a) Completed: **17**
(b) Ongoing: **5**

Number of Postdoctoral Students:

(a) Completed: **2**
(b) Ongoing: **0**

Number of Projects:

(a) Completed: 14
(b) Ongoing: 0

Complete list of publications

1. Books, monographs etc. published

i. A. Pramanik, S. Ghoshal, S. Biswas, B. Rajbanshi, and **P. Sarkar** (**2024**), "Accurate Determination of Materials Properties: Role of Electron Density" contributed book chapter in "*Electron Density: Concepts, Computation and DFT Applications*", ISBN: 978-1-394-21762-5, Wiley.

ii. **P. Sarkar** and S.P. Bhattacharyya (**2022**), "Understanding Properties of Atoms, Molecules and Materials" ISBN: 9781000504439, 1000504433, Book, CRS Press, Taylor and Francis.

iii. A. Pramanik, S. Ghoshal, and **P. Sarkar** (**2022**), "Designing nanoclusters for catalytic activation of small molecules: a theoretical endeavor" contributed book chapter in "*Atomic Clusters with Unusual Structure, Bonding and Reactivity: Theoretical Approaches, Computational Assessment and Applications"*, ISBN: 9780128229439, Elsevier Science Publishing Co Inc.

iv. A. Pramanik, S. Sarkar and **P. Sarkar**, (**2020**), "Charge transport through nanocontacts", invited book chapter in *"Chemical Modelling: Applications and Theory"*, Royal Society of Chemistry, **Vol. 15**, pp. 70–130.

v. S. Sarkar, S. Saha, S. Pal and **P. Sarkar**, (**2016**), "Exploring the electronic structure of nanohybrid materials for their application in solar cell", invited book chapter in *"Chemical Modelling: Applications and Theory"*, Royal Society of Chemistry, **Vol. 13**, pp. 27–71.

vi. S. Pal, S. Sarkar, S. Saha and **P. Sarkar**, (**2012**), "Size-dependent electronic structure of semiconductor nanoparticles", invited book chapter in *"Chemical Modelling: Applications and Theory"*, Royal Society of Chemistry, **Vol. 9**, pp. 135–67.

vii. S. Pal and **P. Sarkar**, (**2010**), "Size and shape dependent structural and electronic properties of metal chalcogenide nanoclusters", invited book chapter in *"Aromaticity and Metal Clusters"*, Editor: P. K. Chattaraj, Taylor and Francis, **October, 15**, pp. 225–241.

2. Research publications in journals

1. U. Chowdhury, S. Mondal, S. Dey, Md Habib, R. Sarkar, S. Gumber, P. Chattopadhyay, **P. Sarkar**, O. Prezhdo, S. Pal, (**2025)** "Hard–Soft Acid–Base Theory Explains Photoexcited Carrier Dynamics in Porphyrin/CNT Nanohybrids: Time-Domain Atomistic Analysis", J. Am. Chem. Soc., 147, 20748.

2. D. Maji, A. Ghosh, D. Barman and **P. Sarkar, (2025)** *"* Accelerating Molecular Dynamics with a Graph Neural Network: A Scalable Approach through E (q) C-GNN", J. Phys. Chem. Lett, 16, 2254.

3. P. Das, A. Ghosh, B. Goswami, and **P. Sarkar, (2025)** *"*Theoretical investigation of a C2N monolayer as a bifunctional electrocatalyst for rechargeable non-aqueous Li–air batteries*",* J Mat. Chem. A , 13, 6376.

4. S. Ghosal and **P. Sarkar, (2025)** "Active Sites Identification on Defect-Engineered TiO2 Surfaces for Ethylene Hydrogenation via DFT and Microkinetics", ChemCatChem, 17, e202500248 (invited Article).

5. A. Ganai and **P. Sarkar, (2025)** "The role of defect-modulated HKUST-1 MOF nodes in non-oxidative ethanol dehydrogenation: an observed phenomenon of catalyst transfiguration" , Dalton Transactions 54 (11), 4599(invited Article).

6. A Mahato, A Mahato, S Ghoshal, A Pramanik, **P Sarkar, (2025**) "Understanding asymmetric hydrogenation of alkenes catalyzed by the first-row transition metal Fe: a first-principles exploration", Phys. Chem. Chem. Phys., 27, 1100.

7. P. Majhi, M. M. Panja, **P. Sarkar** and B. Talukder, (**2025**) "Null Lagrangians in Schwarzian Mechanics", *Phys. Letts. A,* **530,** 130092.

8. P. Das, A. Ghosh and **P. Sarkar**, (**2024**), " Photocarrier Dynamics of Two-Dimensional Aza-Fused Covalent Organic Frameworks as Bifunctional Photocatalysts toward Overall Water Splitting", *ACS Applied Material & Interface*, **16**, 62043.

9. S. Kumar, A. Ghosh and **P. Sarkar**, (**2024**), "Promoting Overall Water Splitting in MoS_2/BSe Heterostructures: Insights from Time-Domain Atomistic Dynamics", *J. Phys. Chem. C*, **128**, 17361.

10. S. Mandal and **P. Sarkar**, (**2024**), "Rattling-Induced Ultralow Lattice Thermal Conductivity Leads to High Thermoelectric Performance in $GaAgSnSe_4$ and $InAgGeSnSe_4$", *ACS Applied Energy Material*, **7**, 9023.

11. S. Kumar, A. Ghosh, S. Pal and **P. Sarkar**, (**2024**), "Controlling the charge carrier dynamics of o-B_2N_2 monolayer through pnictogen family atoms doping", *J. Phys. Chem. Lett.*, **15**, 9388.

12. A. Ganai and **P. Sarkar**, (**2024**), "Computational exploration on coupling formic acid production with propylene synthesis via catalytic transfer hydrogenation: the role of CO_2 beyond reverse water gas shift reaction", *J. Org. Chem.*, **89**, 12010.

13. A. Ghosh, A. Pramanik, S. Pal and **P. Sarkar**, (**2024**), "Emergence of Z-Scheme Photocatalysis for Total Water Splitting: An Improvised Route to High Efficiency", *J. Phys. Chem. Lett.*, **15**, 6841.

14. S. Laru, S. Ghoshal, **P. Sarkar** and A. Hajra, (**2024**), "Unusual regioselective C–H difluoroalkylation of heteroarenes under photoredox catalysis", *Org. Lett.*, **26**, 5098.

15. S. Ghoshal and P. Sarkar, (**2024**), "First-principles insights into the mechanism of CO_2 hydrogenation reactions by Fe-PNP pincer complex", *ChemPhysChem*, e202400425.

16. A. Ganai and **P. Sarkar**, (**2024**), "Unraveling the role of single-atom catalysts immobilized onto metal–organic frameworks in selective acetylene hydrogenation: an implementation of the active site isolation strategy", *J. Phys. Chem. C*, **128**, 7913.

17. P. Das, A. Ghosh and **P. Sarkar**, (**2024**), "Hot carrier controlled nitrogen fixation reaction in metal-free boron-anchored Aza-COF: insight from nonadiabatic molecular dynamics simulation", *J. Phys. Chem. Lett.*, **15**, 4898.

18. A. Ghosh, P. Das, S. Kumar and **P. Sarkar**, (**2024**), "Hot carrier relaxation dynamics of an aza-covalent organic framework during photoexcitation: an insight from ab initio quantum dynamics", *J. Chem. Phys.*, **160**, 164707.

19. S. Chowdhury, **P. Sarkar** and B.C. Gupta, (**2024**), "Can P_3S and C_3S monolayers be used as anode materials in metal-ion batteries? An answer from first-principles study", *Phys. Chem. Chem. Phys.*, **26**, 16240.

20. S. Ghosh, P. Roy, A. Pramanik and **P. Sarkar**, (**2024**), "Photoinduced conductance and carrier switching in homoannulene ester derivatives: a theoretical exploration" *Comput. Theor. Chem.*, 114509.

21. S. Ghoshal and **P. Sarkar**, (**2024**), "Computational screening of suitable adatom to enhance CO_2 electroreduction on noble-metal based dual-atom catalysts", *J. Phys. Chem. C*, **128**, 2392.

22. S. Mandal, A. Ghosh and **P. Sarkar**, (**2024**), "Understanding the origin of the high thermoelectric figure of merit of Zintl-phase KCaBi", *Phys. Chem. Chem. Phys.*, **26**, 13198.

23. A. Ghosh, S. Kumar and **P. Sarkar**, (**2024**), "Point defect-mediated hot carrier relaxation dynamics of lead-free $FASnI_3$ perovskites", *Nanoscale*, **16**, 4737.

24. P. Das, B. Ball and **P. Sarkar**, (**2023**), "Bifunctional electrocatalytic activity of two-dimensional metallophthalocyanine-based metal–organic-frameworks for overall water splitting: a DFT study", *ACS Catal.*, **13**, 16307.

25. A. Ganai and P. **Sarkar**, (**2023**), "Exploring the opportunity of missing linker defect-induced acetic acid synthesis over heterometallic Fe_2M-based metal–organic frameworks", *J. Phys. Chem. C*, **127**, 22049.

26. A. Sarkar, S. Hansda, T. Dutta, S. Ghoshal, S. Mukhopadhyay, **P. Sarkar**, S.K. Mandal, N.C. Saha, P. Chattopadhyay, and K. Dhara, (**2023**), "Endoplasmic reticulum-targeted fluorescent probes for metal-free tracking of carbon monoxide in living cells", *Sensors Actuators B: Chem.*, **393**, 134150.

27. A. Ghosh, B. Goswami, S. Pal and **P. Sarkar**, (**2023**), "How the stacking pattern influences the charge transfer dynamics of van der Waals heterostructures: an answer from a time-domain ab initio study", *J. Phys. Chem. Lett.*, **14**, 7672.

28. S. Saha, S. Ghoshal and **P Sarkar**, (**2023**), "Theoretical exploration of bare and oxygen-functionalized Ti_3C_2 clusters for catalytic NH_3 production", *J. Chem. Sci.*, **135**, 48.

29. P. Das, B. Ball, B. Goswami and **P. Sarkar**, (**2023**), "Designing dithiolene and bis(iminothiolato)-based 1D metal-organic-frameworks for electrocatalytic hydrogen evolution reaction", *Theor. Chem. Acc.*, **142**, 41.

30. P. Das and **P. Sarkar**, (**2023**), "A nitrogen-rich two dimensional covalent organic framework with multiple carbonyls as a highly efficient anchoring material for lithium–sulfur batteries", *Phys. Chem. Chem. Phys.*, **25**, 30536.

31. P. Roy, S. Ghoshal, A. Pramanik and P. **Sarkar**, (**2023**), "Single B-vacancy enriched α1-borophene sheet: an efficient metal-free electrocatalyst for CO_2 reduction", *Phys. Chem. Chem. Phys.*, **25**, 25018.

32. S. Mandal and **P. Sarkar**, (**2023**), "Physical insights into the ultralow lattice thermal conductivity and high thermoelectric performance of bulk LiMTe2 (M= Al, Ga)", *J. Mater. Chem. C*, **11**, 13691.

33. A. Ganai, B. Ball and **P. Sarkar**, (**2023**), "Modulating the energetics of C–H bond activation in methane by utilizing metalated porphyrinic metal–organic frameworks", *J. Phys. Chem. Lett.*, **14**, 1832.

34. S. Mandal and **P. Sarkar**, (**2023**), "Computational exploration of ultralow lattice thermal conductivity and high figure of merit in *p*-type bulk RbX_2Sb (X = K, Na)", *ACS Appl. Energy Mater.*, **2**, 939.

35. S. Ghoshal, A. Ghosh, P. Roy, B. Ball, A. Pramanik and **P Sarkar**, (**2022**), "Recent progress in computational design of single-atom/cluster catalysts for electrochemical and solar-driven N_2 fixation", *ACS Catal.*, **12**, 15541.

36. S. Sannigrahi, A. Ghosh, B. Ball and P. Sarkar, (**2022**), "Exploring Ti_2CO_2-WSe_2 heterostructure as a direct Z-scheme photocatalyst for water splitting: A non-adiabatic study", *J. Phys. Chem. C*, **126**, 20852.

37. S. Ghoshal, P. Roy, A. Pramanik and **P. Sarkar**, (**2022**), "Ru/Rh catalyzed selective hydrogenation of CO_2 to formic acid: a first principles microkinetic analysis", *Catal. Sci. Technol.,* **12**, 7219.

38. A. Ghosh, B. Ball, S. Pal and **P. Sarkar**, (**2022**), "Ultrafast charge transfer and delayed recombination in graphitic-CN/WTe_2 van-der Waals heterostructure: a time domain ab-initio study", *J. Phys. Chem. Lett.*, **13**, 7898.

39. O. Chatterjee, R. Roy, A. Pramanik, T. Dutta, V. Sharma, **P. Sarkar** and A.L. Koner, (**2022**), "Dynamic self-assembly of photo-reduced perylene diimide: single-component white light emission from organic radicals", *Adv. Optical Mater.*, 2201187.

40. P. Das, B. Ball and **P. Sarkar**, (**2022**), "Theoretical investigation of a tetrazine based covalent organic framework as a promising anode material for sodium/calcium ion batteries", *Phys. Chem. Chem. Phys.*, **24**, 21729.

41. S. Mandal, B.A. Khan and **P. Sarkar**, (**2022**), "2D lead free ruddlesden-popper phase perovskites as efficient photovoltaic materials: a first-principles investigation', *Comput. Mater. Sci.*, **211**, 111545.

42. A. Ghosh, S. Mandal and **P. Sarkar**, (**2022**), "2D homogeneous holey carbon nitride: an efficient anode material for Li-ion batteries with ultrahigh capacity', *ChemPhysChem*, e202200182P (invited article).

43. A. Ghosh, S. Pal and **P. Sarkar**, (**2022**), "Rational design of two-dimensional porous boron phosphide as efficient cathode material for Li and Na ion batteries: a first-principles study", *J. Phys. Chem. C*, **126**, 5092.

44. P. Roy, A. Pramanik and **P. Sarkar**, (**2022**), "Polaron induced conductance switching in conjugated oligophenylene: a first-principles analysis", *J. Phys. Chem. A*, **126**, 318.

45. B. Ball, P. Das and **P. Sarkar**, (**2021**), "Molybdenum atom-mediated salphen-based covalent organic framework as a promising electrocatalyst for the nitrogen reduction reaction: a first-principles study", *J. Phys. Chem. C*, **125**, 26061.

46. P. Roy, A. Pramanik and **P. Sarkar**, (**2021**), "Dual-silicon-doped graphitic carbon nitride sheet: an efficient metal-free electrocatalyst for urea synthesis", *J. Phys. Chem. Lett.*, **12**, 10837.

47. M. Kar, A. Ghosh, R. Sarkar, S. Pal and **P Sarkar**, (**2021**), "Arene and functionalized arene based two dimensional organic–inorganic hybrid perovskites for photovoltaic applications", *J. Comput. Chem.*, **42**, 1982.

48. A. Ghosh, M. Kar, C. Majumder and **P. Sarkar**, (**2021**), "First-principles calculations to investigate electronic structure and transport properties of CrC monolayers: a new horizon for spintronic application", *Mater. Sci. Eng.: B*, **272**, 115379.

49. S. Mukhopadhyay, A. Sarkar, S. Ghoshal, **P. Sarkar**, K. Dhara and P. Chattopadhyay, (**2021**), "Encapsulation and stabilization of a donor–acceptor stenhouse adduct isomer in water inside the blue box: a combined experimental and theoretical approach", *J. Phys. Chem. B*, **125**, 7222.

50. B. Ball and **P. Sarkar** (**2021**), "Tuning the structural skeleton of a phenanthroline-based covalent organic framework for better electrochemical performance as a cathode material for Zn-ion batteries: a theoretical exploration", *Phys. Chem. Chem. Phys*., **23**, 12644.

51. R. Sarkar, M. Kar, M. Habib, G. Zhau, Th. Frauenheim, **P. Sarkar**, S. Pal and O.V. Prezhdo (2021), "Common defects accelerate charge separation and reduce recombination in CNT/molecule composites: atomistic quantum dynamics", *J. Am. Chem. Soc.,* **143**, 6649.

52. A. Chowdhury, S. Biswas, S. Ghoshal, A. Pramanik and **P. Sarkar**, (**2021**), "Photo-redox coupled Co-pincer complexes for efficient decarbonylation of aryl carbonyls: a quantum chemical investigation", *Mol. Catal.*, **507**, 111553.

53. P. Roy, A. Pramanik and **P. Sarkar**, (**2021**), "Graphitic carbon nitride sheet supported single-atom metal-free photocatalyst for oxygen reduction reaction: a first principles analysis", *J. Phys. Chem. Lett.*, **12**, 2788.

54. A. Ghosh, M. Kar, C. Majumder and **P. Sarkar**, (**2021**), "Half metallicity and ferromagnetism of vanadium nitride nanoribbons: a first-principles study", *Phys. Chem. Chem. Phys.*, **23**, 1127.

55. S. Ghoshal, A. Pramanik and **P. Sarkar**, (**2021**), "Towards H_2O catalyzed N_2-fixation over TiO_2 doped Ru_n clusters (n= 5, 6): a mechanistic and kinetic approach", *Phys. Chem. Chem. Phys.*, **23**, 1527.

56. M. Kar, R. Sarkar, S. Pal and **P. Sarkar**, (**2021**), "Lead free two-dimensional mixed tin and germanium halide perovskites for photovoltaic applications", *J. Phys. Chem. C*, **125**, 74.

57. B. Ball, B.A. Khan, B. Goswami and **P. Sarkar**, (**2020**), "Conductance switching of a gold-covalent organic framework nanojunction via proton transfer", *Phys. Lett. A*, **389**, 127100.

58. M. Kar, R. Sarkar, S. Pal and **P. Sarkar**, (**2020**), "Tunable electronic structure of two-dimensional MoX_2 (X=S, Se)/SnS_2 van der Waals heterostructures", *J. Phys. Chem. C*, **124**, 21357.

59. B. Ball and **P. Sarkar**, (**2020**), "Triazine-and keto-functionalized porous covalent organic framework as a promising anode material for Na-ion batteries: a first-principles study", *J. Phys. Chem. C*, **124**, 15870.

60. S. Ghoshal, A. Pramanik and **P. Sarkar**, (**2020**), "Theoretical investigations on the possibility of prebiotic HCN formation via O-addition reactions", *J. Phys. Chem. A*, **124**, 4782.

61. M. Kar, S. Sarkar and **P. Sarkar**, (**2020**), "Highly efficient inorganic-organic heterojunction solar cells based on polymer and CdX (X= Se, Te) quantum dots: an insight from a theoretical study", *J. Phys. Chem. C*, **124**, 11350.

62. M. Kar, R. Sarkar, S. Pal and **P. Sarkar**, (**2020**), "Two dimensional CP_3 monolayer and its fluorinated derivative with promising electronic and optical properties: a theoretical study", *Phys. Rev. B*, **101**, 195305.

63. N.N. Ghosh, S. Saha, A. Pramanik, **P. Sarkar** and S. Pal, (**2020**), "Molecular design of porphyrin dyes using different electron-withdrawing moieties for high performance dye-sensitized solar cells", *Comput. Theor. Chem.*, **1182**, 112846.

64. M. Kar, S. Saha, R. Sarkar, S. Pal and **P. Sarkar**, (**2020**), "A Comparative Study on the Photovoltaic Properties of ZnX (X= S, Se, Te) QD/CNT Inorganic/Organic Hybrid Nanocomposites", *J. Phys. Chem. C*, **124**, 7652.

65. R. Sarkar, M. Habib, M. Kar, A. Pramanik, S. Pal and **P. Sarkar**, (**2020**), "Structural rigidity accelerates quantum decoherence and extends carrier lifetime in porphyrin nanoball: a time domain atomistic simulation", *Nanoscale Adv.*, **2**, 1502.

66. B. Ball, C. Chakravarty and **P. Sarkar**, (**2020**), "Silicon and phosphorous co-doped bipyridine-linked covalent triazine framework as a promising metal-free catalysts for hydrogen evolution reaction: a theoretical investigation", *J. Phys. Chem. Lett.*, **11**, 1542.

67. C. Chakravarty, B. Mandal, and **P. Sarkar**, (**2020**), "Bis (iminothiolato)-based one dimensional metal-organic framework: robust bipolar magnetic semiconductor with reversal of spin-polarization", *J. Phys. Chem. C*, **124**, 37.

68. B. Ball, C. Chakravarty and **P. Sarkar**, (**2019**), "Two-dimensional covalent triazine framework as a promising anode material for Li-Ion batteries', *J. Phys. Chem. C*, **123**, 30155.

69. G. Zhang, F. Hermerschmidt, A. Pramanik, D. Schollmeyer, M. Baumgarten, **P. Sarkar**, E. J. W. List-Kratochvil and K. Mllen, (**2019**), "Bulky, dendronized iridium complexes and their photoluminescence", *J. Mater. Chem. C*, **7**, 15252.

70. S. Ghoshal, A. Pramanik, S. Biswas and **P. Sarkar**, (**2019**), "CH_3NO as a potential intermediate for early atmospheric HCN: a quantum chemical insight", *Phys. Chem. Chem. Phys.*, **21**, 25126.

71. A. Chowdhury, S. Biswas, A. Pramanik and **P. Sarkar**, (**2019**), "Mechanistic insights into the non-bifunctional hydrogenation of ester by Co(II) pincer complexes: a DFT study", *Dalton Trans.*, **48**, 16083.

72. M. Kar, B. Rajbanshi, R. Sarkar, S. Pal and **P. Sarkar**, (**2019**), "Periodically-ordered one and two dimensional CdTe QD superstructures: a path forward in photovoltaics", *Phys. Chem. Chem. Phys.*, **21**, 19391.

73. M. Habib, M. Kar, S. Pal and **P. Sarkar**, (**2019**), "The role of chalcogens in the exciton relaxation dynamics of chalcogenol functionalized CdSe QD: a time-domain atomistic simulation", *Chem. Mater.*, **31**, 4042.

74. M. Kar, R. Sarkar, S. Pal and **P. Sarkar**, (**2019**), "Edge-modified phosphorene antidot nanoflakes and their van der Waals heterojunctions for solar cell applications", *J. Phys. Chem. C*, **123**, 20748.

75. S. Urinda, G. Das, A. Pramanik and **P. Sarkar**, (**2019**), "Can remote N-heterocyclic carbenes be used for designing efficient blue triplet emitters? An answer from quantum chemical investigation", *J. Phys. Chem. C*, **123**, 14216.

76. N.N. Ghosh, M. Habib, A. Pramanik, **P. Sarkar** and S Pal, (**2019**), "Molecular engineering of anchoring groups for designing efficient triazatruxene-based organic dye-sensitized solar cells", *New J. Chem.,* **43**, 6480.

77. M. Habib, R. Sarkar, S. Biswas, A. Pramanik, **P. Sarkar** and S. Pal, (**2019**), "Unambiguous hydrogenation of CO_2 by coinage-metal hydride anions: an intuitive idea based on *in-silico* experiments", *Phys. Chem. Chem. Phys.,* 21, 7483.

78. A. Pramanik, S. Biswas, S. Pal and **P. Sarkar**, (**2019**), "Charge transport and transfer phenomena involving conjugated acenes and heteroacenes", *Bull. Mater. Sci.*, **42**, 128.

79. B. Ball, C. Chakravarty, B. Mandal and **P Sarkar**, (**2019**), "Computational investigation on the electronic structure and functionalities of a thiophene-based covalent triazine framework", *ACS Omega*, **4**, 3556.

80. M. Kar, R. Sarkar, S. Pal and **P. Sarkar**, (**2019**), "Pathways for improving the photovoltaic efficiency of porphyrin and phosphorene antidot lattice nanocomposite: an insight from theoretical study", *J. Phys. Chem. C*, **123**, 5303.

81. M. Kar, R. Sarkar, S. Pal and **P. Sarkar**, (**2019**), "Engineering the magnetic properties of $PtSe_2$ monolayer through transition metal doping", *J. Phys.: Condensed Matter*, **31**, 145502.

82. S. Urinda, G. Das, A. Pramanik and **P. Sarkar**, (**2018**), "Essential role of ancillary ligand in color tuning and quantum efficiency of Ir(III) complexes with N-heterocyclic or mesoionic carbene ligand: a comparative quantum chemical study", *J. Phys. Chem. A,* **122**, 7532.

83. T. Mallick, A. Karmakar, D. Mandal, A. Pramanik, **P. Sarkar** and N.A. Begum, (**2018**) , "Harnessing carbazole based small molecules for the synthesis of the fluorescent gold nanoparticles: a unified experimental and theoretical approach to understand the mechanism of synthesis", *Colloids Surf. B: Biointerfaces*, **172**, 440.

84. M. Habib, N.N. Ghosh, R. Sarkar, A. Pramanik, **P. Sarkar** and S. Pal, (**2018**), "Controlling the charge transfer and recombination dynamics in hollow ZnO QD based dye sensitized solar cell: an insight from ab initio simulation", *Chem. Phys. Lett.*, **709**, 21.

85. P. Roy, S. Biswas, A. Pramanik and **P. Sarkar**, (**2018**), "Substitution induced carrier switching in S,N-heteroacene molecular junctions: a first principle analysis", *Chem. Phys. Lett.*, **708**, 87.

86. S. Biswas, A. Chowdhury, P. Roy, A. Pramanik and **P. Sarkar**, (**2018**), "Computational studies on the hydride transfer barrier for the catalytic hydrogenation of CO_2 by different Ni(II) complexes", *J. Mol. Model. (invited article)*, **24**, 224.

87. S. Biswas, A. Pramanik and **P. Sarkar**, (**2018**), "Origin of different photovoltaic activities in regioisomeric small organic molecule solar cells: the intrinsic role of charge transfer processes", *J. Phys. Chem. C*, **122**, 14296.

88. M. Habib, S. Saha, R. Sarkar, A. Pramanik, **P. Sarkar** and S. Pal, (**2018**), "Computational design of some TTF-substituted acene-based dyes for solar cell application using hollow ZnO quantum dot as acceptor", *Comput. Theor. Chem.*, **1136**, 10.

89. C. Chakravarty, B. Mandal and **P. Sarkar**, (**2018**), "Porous graphene-fullerene nanocomposites: a new composite for solar cell and optoelectronic applications", *J. Phys. Chem. C*, **122**, 15835.

90. S. Biswas, A. Pramanik and **P. Sarkar**, (**2018**), "Computational design of quaterpyridinebased Fe/Mn-complexes for the direct hydrogenation of CO_2 to HCOOH: a direction for atom-economic approach", *ChemistrySelect*, **3**, 5185.

91. M. Kar, B. Rajbanshi, S. Pal and **P. Sarkar**, (**2018**), "Engineering the electronic structure of tin sulfide nanoribbons: a computational study", *J. Phys. Chem. C*, **122**, 5731.

92. C. Chakravarty, B. Mandal and **P. Sarkar**, (**2018**), "Multi-functionalities of an azine-linked covalent-organic framework: from nanoelectronics to nitro-explosive detection and conductance switching", *J. Phys. Chem. C*, **122**, 3245.

93. N.N. Ghosh, M. Habib, A. Pramanik, **P. Sarkar** and S. Pal., (**2018**), "Tuning the BODIPY core for its potential use in DSSC: a quantum chemical approach", *Bull. Mater. Sci.*, **41**, 56.

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