

PROFILE

Name: **Ngangbam Bedamani Singh**
Father's name: Ngangbam Budhichandra Singh
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❖ Area of Interest

- Computational simulation methods, density functional theory, molecular dynamics.
- Structure, bonding and reactivity of metal cluster.
- 2-D materials such as graphene, Graphene, borophene, etc.
- Designing materials for clean energy (Hydrogen storage, solar energy, metal-ion Batteries)

❖ Education and Qualifications

Ph. D.	2015
Assam University, Silchar, India	
Master of Science, Physics (Specialization: Condensed Matter Physics)	2008 70.69%
Assam University, Silchar, India	

❖ Publication Details

a. Publication in National/International Journals

- 1) *Density Functional Theory Studies of van der Waals Heterostructures Comprised of MoSi₂P₄ and BAs Monolayers for Solar Cell Applications*
Ngangbam Bedamani Singh, Rajkumar Mondal, Jyotirmoy Deb, Debolina Paul, Utpal Sarkar (2024) ACS Appl. Nano Mater. 7: 6704–6711.
- 2) *Electronic and transport property of two-dimensional boron phosphide sheet*,
Rajkumar Mondal, **Ngangbam Bedamani Singh**, Jyotirmoy Deb, Swarnakamal Mukherjee, Utpal Sarkar (2022) Journal of Molecular Graphics and Modelling **112**, 108117.
- 3) *Theoretical study of electronic transport through P-porphyrin and S-porphyrin nanoribbons*,
R Mondal, B Bhattacharya, **Ngangbam Bedamani Singh**, Utpal Sarkar (2020) Journal of Molecular Graphics and Modelling **97**, 107543.

- 4) *First principle study of adsorption of boron halogenated system on pristine graphene*, Jyotirmoy Deb, Barnali Bhattacharya, **Ngangbam Bedamani Singh**, Utpal Sarkar (2016) *Structural Chemistry*, **27**/1-4.
- 5) *Electronic and optical properties of pristine and boron-nitrogen doped graphyne nanotubes*, Barnali Bhattacharya, **Ngangbam Bedamani Singh**, Rajkumar Mondal, Utpal Sarkar (2015) *Phys Chem Chem Phys* **17**, 19325-19341.
- 6) *NO adsorption on nickel and nickel-manganese bimetallic clusters: A density functional study*, **Ngangbam Bedamani Singh**, B Indrajit Sharma, Utpal Sarkar (2015) *Physica E: Low-dimensional systems and Nanostructures* **73**, 12-20.
- 7) *Pristine and BN Doped Graphyne Derivatives for UV Light Protection*, Barnali Bhattacharya, **Ngangbam Bedamani Singh**, Utpal Sarkar (2015) *International Journal of Quantum Chemistry* **115**, 820-829.
- 8) *Emissive bis-salicylaldiminato Schiff base ligands and their zinc(II) complexes: Synthesis, photophysical properties, mesomorphism and DFT studies*, Manoj Kr. Paul, Y. Dilipkumar Singh, **Ngangbam Bedamani Singh**, Utpal Sarkar (2015) *Journal of Molecular Structure* **1081**, 316–328.
- 9) *Nickel cluster functionalised carbon nanotube for CO molecule detection: a theoretical study*, **Ngangbam Bedamani Singh**, Barnali Bhattacharya, Rajkumar Mondal and Utpal Sarkar (2015) *Molecular Physics* **114**, 671-680.
- 10) *Structure, Vibrational and Optical Properties of Platinum Cluster: A Density Functional Theory Approach*, **Ngangbam Bedamani Singh**, Utpal Sarkar (2014) *Journal of Molecular Modeling* **20**, 2537/1-2537/11.
- 11) *A first principle study of pristine and BN-doped graphyne family*, **Ngangbam Bedamani Singh**, Barnali Bhattacharya, Utpal Sarkar (2014) *Structural Chemistry* **25**, 1695-1710.
- 12) *A density functional study of chemical, magnetic and thermodynamic properties of small palladium clusters*, **Ngangbam Bedamani Singh**, Utpal Sarkar (2014) *Molecular Simulation* **40**, 1255-1264.

b. Publication in Conference Proceedings

- 1) *Tuning the magnetic property of vacancy defected graphyne by transition metal absorption*, Barnali Bhattacharya, **Ngangbam Bedamani Singh**, Utpal Sarkar (2015) *AIP Conf. Proc.* **1665**, 050066. (UGC APPROVED) (impact factor 0.402) (ISSN **1551-7616**)
- 2) *Tuning of band gap due to fluorination of graphyne and graphdiyne*, Barnali Bhattacharya, **Ngangbam Bedamani Singh**, Utpal Sarkar (2014) *Journal of Physics: Conference Series* **566**, 012014/1-5. (UGC APPROVED) (impact factor 0.48) (ISSN **1742-6588**)

3) *A computational study of armchair nanotube*, **Ngangbam Bedamani Singh**, Utpal Sarkar (2012) AIP Conf. Proc. **1461**, 241-245. (UGC APPROVED) (impact factor 0.402) (ISSN **1551-7616**)

c. Publication in Book Chapter

1) *Nanoelectronic Application of Graphyne and Its Structural Derivatives*

B Bhattacharya, **Ngangbam Bedamani Singh**, Utpal Sarkar (2019) HANDBOOK OF GRAPHENE Vol.3 chapter 5 (page 151-176). (ISBN:9781119459903 |Online ISBN:9781119468455) DOI:10.1002/9781119468455 Publisher: John Wiley & Sons, Inc., 111 River Street, Hoboken, NJ 07030, USA and Scrivener Publishing LLC, 100 Cummings Center, Suite 541J, Beverly, MA 01915, USA © 2019 Scrivener Publishing LLC



Seminar/Conference/Workshop/School attended

- 1) Lecture delivered on the topic “**Two-Dimensional BeB₂ as a potential anode material for Mg-ion batteries**” in “*International conference on systems and processes in physics, chemistry, and biology ICSPPCB-2023*” organized by Department of Physics, Assam University Silchar on 2-4 March, 2023.
- 2) Lecture delivered on the topic “**First principles analysis of borophene and borophane**” in “*International conference on systems and processes in physics, chemistry, and biology ICSPPCB-2018*” organized by Department of Physics, Assam University Silchar on 1-3 March, 2018.
- 3) Attended “National Workshop on Atomistic Simulation Techniques for Material Science, Nano Technology and Biosciences (NWASt-2015)” held during 21-24 December, 2015 at Indian Institute of Technology, Guwahati.
- 4) Participated in “3 days workshop on Microwave: Basics and applications” held at Department of Physics, Assam University, Silchar, 25-27 July, 2014.
- 5) Participated in the “Summer School on Materials Simulation Theory and Numerics (MASTANI)” organized by Indian Institute of Science and Educational Research, Pune in collaboration with “The Abdus Salam International Centre for theoretical Physics” held during 30 June-12 July, 2014.
- 6) Participated in the “National Symposium on Clusters, Cluster assemblies and nano-scale materials (ISCANM-III)” held during 11-14 March, 2014 at Harish Chandra Research Institute Allahabad, India.

- 7) Participated in the “Lecture series on nanoscience and technology” organized at Department of Physics, Assam University, Silchar, 16-18 January, 2014.
- 8) Attended “Science Academies’ Refresher course in theoretical physics” held at Department of Physics, Assam University, Silchar, 2-15 December, 2013.
- 9) Presented a poster entitled “**Nickel Decorated Single-Wall Carbon Nanotube as CO Sensor**” in “Indo-US International Workshop on Nanosensor Science & Technology (IWNST-2013)” organized by National Institute of Science and Technology, Berhampur, Orissa during 27 February-1 March, 2013.
- 10) Presented a poster entitled “**Single Walled Armchair Carbon Nanotube**” in “National Seminar on Emerging Areas of Research & Development in Chemical and Physical Sciences in North East India” held at Srikishan Sarada College, Hailakandi, 16-18 October, 2012.
- 11) Presented a poster entitled “**A Computational Study of armchair carbon nanotube**” in the “International Workshop on Functional Materials, IWFM-2011” organized by National Institute of Science and Technology, Berhampur, India in collaboration with Drexel University, Philadelphia, U.S.A., during 20-22 December, 2011.
- 12) Presented a poster entitled “**Computational Study of Reactivity profile of armchair carbon nanotube**” in the “Diamond Jubilee Symposium on Recent Trends in Chemistry (DJSRTC-2011)” held at Department of Chemistry, Indian Institute of Technology Kharagpur during 21-23 October, 2011.
- 13) Presented a poster entitled “**Studies on the structure and properties of small palladium clusters using density functional theory**” in the “One Day National Workshop on Soft Materials” held on 17 September, 2011 at Centre for Soft Matter, Department of Chemistry, Assam University, Silchar.
- 14) Participated in the “National Workshop on Computational Physics” held during 14-19 February, 2011 at Department of Physics, Mizoram University.
- 15) Participated in the “Winter School on Gravitation and Cosmology, 2011” organized by Department of Physics, Assam University, Silchar on 5-11 February, 2011.
- 16) Lecture delivered on the topic “**Study on structure and properties of some platinum clusters using density functional theory**” in “National Seminar on Current Trends in Condensed Matter Physics (CTCMP-2011)” organized by Department of Physics, Assam University Silchar on 3-5 February, 2011.

Dr. Ngangbam Bedamani Singh