

# Harikrishna Sahu

## Curriculum Vitae

Research Scientist II  
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## CAREER OBJECTIVE

My career objective is to become a professor at a renowned university, where I can blend my passion for research with the joy of teaching. I aspire to contribute to the academic community through innovative research endeavors and inspire the next generation of learners while fostering a culture of intellectual curiosity and knowledge dissemination.

## SUMMARY OF QUALIFICATION

- Have five years of post-PhD research experience with a strong publication record.
- Develop and use computational and machine learning tools to investigate organic materials.
- Have experience working collaboratively with industry (Toyota Research Institute, Los Altos, CA).
- Have experience in writing proposals to acquire computational resources.

## EDUCATION

| Degree        | Specialization          | University/College/Board        | Year | % or CGPA  |
|---------------|-------------------------|---------------------------------|------|------------|
| Matriculation | NA                      | BSE, Odisha                     | 2004 | 73.47%     |
| XII Class     | NA                      | CHSE, Odisha                    | 2006 | 63.11%     |
| B.Sc.         | Chemistry               | North Orissa University, Odisha | 2009 | 72.5%      |
| M.Sc.         | Chemistry               | NIT Rourkela, Odisha            | 2011 | 8.88/10.00 |
| Ph.D.         | Computational chemistry | IIT Guwahati, Assam             | 2016 | 7.23/10.00 |

Details of **Thesis Title:** *In-silico* investigation of optical and electronic properties of hetero-cyclic conjugated polymers.

**Supervisor:** Aditya N. Panda

Date of Joining of Ph.D. program: 21-07-2011

Date of Defence of Ph.D. Thesis: 24-10-2016

- All foreign academic qualifications, earned through education completed outside the United States, have been evaluated by Academic Evaluation Services, Inc., a reputable member firm of NACES (National Association of Credential Evaluation Services).

## RESEARCH INTERESTS

### Developing and applying machine learning and computational tools for designing organic materials.

- Developing active learning pipelines for discovering small molecules or polymers with targeted performance.
- Developing practical tool-kits to construct a hierarchy of polymer models.
- Developing machine-learning (ML) models for predicting the properties of organic materials and screening of hypothetical candidates.
- Interpreting ML models using Shapley Additive exPlanations (SHAP) and z-score analyses, followed by exploring guidelines for designing polymers.
- Studying structural and optoelectronic properties of organic materials using density functional theory (DFT).

## PROFESSIONAL EXPERIENCE

- 05/2023-present **Research Scientist II**, Georgia Institute of Technology, USA.  
**Supervisor:** Rampi Ramprasad  
**Research Topic:** Develop and apply computational and machine learning tools to accelerate materials discovery
- 09/2019-05/2023 **Postdoc**, Georgia Institute of Technology, USA.  
**Supervisor:** Rampi Ramprasad  
**Research Topic:** Develop and apply computational and machine learning tools to accelerate materials discovery
- 03/2017-06/2019 **Postdoc**, Nanjing University, China.  
**Supervisor:** Haibo Ma  
**Research Topic:** Designing organic materials for solar cell applications using machine learning

## PUBLICATIONS (Citations as per Google Scholar)

- 14 Mingzhe Li, Liang Yue, Arunkumar Chitteth Rajan, Luxia Yu, **Harikrishna Sahu**, S. Macrae Montgomery, Rampi Ramprasad, and H. Jerry Qi, Low temperature 3D printing of transparent silica glass microstructures, *Sci. Adv.*, 9, eadi2958 **2023**, DOI: 10.1126/sciadv.adi2958; **IF: 13.6; CITED BY : 0.**
- 13 **Harikrishna Sahu**, Kuan-Hsuan Shen, Joseph H. Montoya, Huan Tran and Rampi Ramprasad, Polymer Structure Predictor (PSP): A Python Toolkit for Predicting Atomic-Level Structural Models for a Range of Polymer Geometries, *J. Chem. Theory Comput.*, 18, 2737, **2022**, DOI: 10.1021/acs.jctc.2c00022; **IF: 6.578; CITED BY : 6.**
- 12 Elyas Abbasi Jannat Abadi, **Harikrishna Sahu**, Seyed Morteza Javadpour, Masoud Goharimanesh, Interpretable Machine Learning for Developing High-Performance Organic Solar Cells, *Mater. Today Energy*, 25, 100969, **2022**, DOI: 10.1016/j.mtener.2022.100969; **IF: 9.257; CITED BY : 7.**

- 11 Rishi Gurnani, Deepak Kamal, Huan Tran, **Harikrishna Sahu**, Kenny Scharm, Usman Ashraf, and Rampi Ramprasad, polyG2G: A Novel Machine Learning Algorithm Applied to the Generative Design of Polymer Dielectrics, *Chem. Mater.*, 33, 7008, **2021**, DOI:10.1021/acs.chemmater.1c02061; IF: 10.508; CITED BY : 18.
- 10 Chao Wu, Lihua Chen, Ajinkya Deshmukh, Deepak Kamal, Zongze Li, Pranav Shetty, Jierui Zhou, **Harikrishna Sahu**, Huan Tran, Gregory Sotzing, Rampi Ramprasad, and Yang Cao, Dielectric Polymers Tolerant to Electric Field and Temperature Extremes: Integration of Phenomenology, Informatics, and Experimental Validation, *ACS Appl. Mater. Interfaces*, 13, 53416, **2021**, DOI: 10.1021/acsami.1c11885; IF: 10.383; CITED BY : 17 .
- 9 **Harikrishna Sahu**, Hongmo Li, Lihua Chen, Arunkumar Chit-teth Rajan, Natalie Stingelin and Rampi Ramprasad, An Informatics Approach for Designing Conducting Polymers, *ACS Appl. Mater. Interfaces*, 13, 53314, **2021**, DOI: 10.1021/acsami.1c04017; IF: 10.383; CITED BY : 8.
- 8 **Harikrishna Sahu** and Haibo Ma, Unraveling Correlations between Molecular Properties and Device Parameters of Organic Solar Cells Using Machine Learning, *J. Phys. Chem. Lett.*, 10, 7277, **2019**, DOI: 10.1021/acs.jpcllett.9b02772; IF: 6.888; CITED BY : 66 .
- 7 **Harikrishna Sahu**, Feng Yang, Xiaobo Ye, Jing Ma, Weihai Fang and Haibo Ma, *Designing Promising Molecules for Organic Solar Cells via Machine Learning Assisted Virtual Screening*, *J. Mater. Chem. A*, 7, 17480, **2019**, DOI: 10.1039/C9TA04097H; IF: 14.511; CITED BY : 83 .
- 6 **Harikrishna Sahu**, Weining Rao, Alessandro Troisi, and Haibo Ma, Toward Predicting Efficiency of Organic Solar Cells via Machine Learning and Improved Descriptors, *Adv. Energy Mater.*, 8, 1801032, **2018**, DOI: 10.1002/aenm.201801032; IF: 29.698; CITED BY : 157 .
- 5 **Harikrishna Sahu**, Rishabh Shukla, Juri Goswami, Priyank Gaur, and Aditya N. Panda, Alternating Phenylene and Furan/Pyrrole/Thiophene Units-based Oligomers: A Computational Study of the Structures and Optoelectronic Properties, *Chem. Phys. Lett.*, 692, 152, **2018**, DOI: 10.1016/j.cpllett.2017.12.034; IF: 2.719; CITED BY : 5 .
- 4 **Harikrishna Sahu** and Aditya N. Panda, Helical and Nonhelical Structures of Vinylene- and Azomethine-Linked Heterocyclic Oligomers: A Computational Study of Conformation-Dependent Optoelectronic Properties, *J. Phys. Chem. C*, 119, 22855, **2015**, DOI: 10.1021/acs.jpcc.5b08100; IF: 4.177; CITED BY : 7 .
- 3 **Harikrishna Sahu**, Shashwat Gupta, Priyank Gaur and Aditya N. Panda, Structure and Optoelectronic Properties of Helical Pyridine-Furan, Pyridine-Pyrrole and Pyridine-Thiophene Oligomers, *Phys. Chem. Chem. Phys.*, 17, 20647, **2015**, DOI: 10.1039/C5CP02872H; IF: 3.945; CITED BY : 21 .

- 2 **Harikrishna Sahu** and Aditya N. Panda, Computational Investigation of Charge Injection and Transport Properties of a Series of Thiophene–Pyrrole based Oligo-Azomethines, *Phys. Chem. Chem. Phys.*, 16, 8563, **2014**, DOI: 10.1039/C3CP55243H; IF: 3.945; CITED BY : 64 .
- 1 **Harikrishna Sahu** and Aditya N. Panda, Computational Study on the Effect of Substituents on the Structural and Electronic Properties of Thiophene–Pyrrole-Based  $\pi$ -Conjugated Oligomers, *Macromolecules*, 46, 844, **2013**, DOI: 10.1021/ma3024409; IF: 6.057; CITED BY : 38 .

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## WORKSHOPS/SCHOOLS

- 2019 **Responsible Conduct of Research (RCR) training**, Hosted by Georgia Tech, Atlanta, USA, October 23 – 24.
- 2017 **Machine Learning in the Molecular Science**, Hosted by NYU-ECNU, Shanghai, China, June 12 – 16.
- 2014 **National Workshop on Molecular Modeling and Simulation of Sustainable Polymers and Nanocomposites (MSSP)**, Hosted by Department of Chemical Engineering, IIT Guwahati, India, August 4 – 8.
- 2014 **DST–SERB Winter School on Modeling Chemical and Biological (Re)activity (MCBR)** , Hosted by International Institute of Information Technology, Hyderabad, India, January 2 – 22.

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## CONFERENCE PRESENTATIONS (ORAL)

- 1 **Harikrishna Sahu**, Huan Tran, Kuan-Hsuan Shen, Joseph Montoya and Rampi Ramprasad, PSP: A toolkit for efficient generation of 3D atomic-level polymer models, *MRS Fall*, hosted by Materials Research Society, USA, Dec. 6-8, **2021**.
- 2 **Harikrishna Sahu**, Huan Tran, Kuan-Hsuan Shen, Joseph Montoya and Rampi Ramprasad, PSP: A toolkit for efficient generation of 3D atomic-level polymer models, *ACS Fall*, hosted by American Chemical Society, USA, Aug. 22-26, **2021**.
- 3 Huan Tran, **Harikrishna Sahu**, Beatriz Gonzalez Del Rio, Deepak Kamal, Chiho Kim, Rampi Ramprasad, An Autonomous Computational Workflow for Efficient Generation of Polymer Data, *Virtual AIChE Annual Meeting*, Nov. 18, **2020**.
- 4 **Harikrishna Sahu**, Feng Yang, Xiaobo Ye, Jing Ma, Weihai Fang, and Haibo Ma, Designing promising molecules for organic solar cells via machine learning assisted virtual screening, *The 6th Asian Materials Data Symposium (AMDS 2019)*, hosted by Materials Genome Institute, Shanghai University, China, Apr. 15-18, **2019**.
- 5 **Harikrishna Sahu** and Aditya N. Panda, Linear and folding conformers of vinylene-, azomethine-, and azo-linked heterocyclic oligomers: Stabilities and optoelectronic properties, *Research Conclave*, hosted by Indian Institute of Technology Guwahati, Assam, Mar. 23-26, **2015**.

## CONFERENCE PRESENTATIONS (POSTER)

- 1 Keara Frawley, **Harikrishna Sahu**, Naresh Thadhani, and Rampi Ramprasad, Predicting Velocimetry Curves from Photonic Doppler Velocimetry (PDV) Signals using Neural Networks, *22nd Biennial Conference of the APS Topical Group on Shock Compression of Condensed Matter*, Anaheim, California, Jul. 11-15, **2022**.
- 2 **Harikrishna Sahu**, Huan Tran, Kuan-Hsuan Shen, Joseph Montoya and Rampi Ramprasad, PSP: A toolkit for efficient generation of 3D atomic-level polymer models, *Advanced Research Computing (ARC) Symposium*, hosted by Georgia Institute of Technology, USA, Nov. 17, **2021**.
- 3 **Harikrishna Sahu**, Huan Tran, Kuan-Hsuan Shen, Joseph Montoya and Rampi Ramprasad, PSP: A toolkit for efficient generation of 3D atomic-level polymer models, *ACS Fall*, hosted by American Chemical Society, USA, Aug. 22-26, **2021**.
- 4 Hongmo Li, **Harikrishna Sahu**, Lihua Chen, Arunkumar Chitteth Rajan, Chiho Kim, Natalie Stingelin, Rampi Ramprasad, An Informatics Approach for Designing Doped Conjugated Polymers, *MRS Fall*, hosted by Materials Research Society, USA, Nov. 30 - Dec. 7, **2021**.
- 5 **Harikrishna Sahu**, Feng Yang, Xiaobo Ye and Haibo Ma, Designing Promising Molecules for Organic Solar Cells via Machine Learning Assisted Virtual Screening, *Frontiers in Chemical Sciences (FICS)*, Indian Institute of Technology Guwahati, Assam, Dec. 6-8, **2018**.
- 6 **Harikrishna Sahu**, Weining Rao, Alessandro Troisi and Haibo Ma, Towards predicting efficiency of organic solar cells via machine learning and improved descriptors, *Gordon Research Conference on Hybrid Electronic and Photonic Materials and Phenomena*, held at Regal Riverside Hotel in Hong Kong, China, Jun. 10-15, **2018**.
- 7 **Harikrishna Sahu**, Shashwat Gupta, Priyank Gaur and Aditya N. Panda, Structural and optoelectronic properties of pyridine-furan, pyridine-pyrrole and pyridine-thiophene helices: A DFT study, *ChemConvenc*, hosted by Indian Institute of Technology Guwahati, Assam, Apr. 8, **2015**.
- 8 **Harikrishna Sahu** and Aditya N. Panda, Structural and Optoelectronic Properties of Linearly and Helically Conjugated Vinylene-linked Heterocyclic Oligomers: A DFT study, *Theoretical chemistry symposium (TCS)*, hosted by CSIR - National Chemical Laboratory, Pune, Dec. 18-21, **2014**.
- 9 **Harikrishna Sahu** and Aditya N. Panda, Thiophene-Pyrrole-based Oligo-Azomethines for Optoelectronic Applications: A Computational Study, *Chemistry with Computers (CWC)*, hosted by IIIT and ICT, Hyderabad, Jan. 18-19, **2014**.
- 10 **Harikrishna Sahu** and Aditya N. Panda, Detailed Investigation on Charge Injection and Transport Properties of a Series of Thiophene-pyrrole-based Oligo-azomethines, *Current Trends in Theoretical Chemistry (CTTC)*, hosted by Bhabha Atomic Research Centre, Mumbai, Sep. 26-28, **2013**.
- 11 **Harikrishna Sahu** and Aditya N. Panda, Electronic structures of thiophene-pyrrole based oligomers in neutral and charged states: A computational study, *Theoretical chemistry symposium (TCS)*, hosted by Indian Institute of Technology Guwahati, Assam, Dec. 19-22, **2012**.

- 12 **Harikrishna Sahu** and Aditya N. Panda, Structural, optical and electronic properties of thiophene and pyrrole based oligomers: A computational study, *Frontiers in Chemical Sciences (FICS)*, hosted by Indian Institute of Technology Guwahati, Assam, Dec. 2-3, **2012**.

## RESEARCH GROUP MANAGEMENT AND SYSTEM ADMINISTRATION

2021-present **In addition to research, I oversee computational and other resources in our research group. Key responsibilities:**

- Write proposals for acquiring computing resources:
  - 3,000,000 ACCESS credits - approved on Feb 21, 2023, for a period of 1 year starting from Apr 01, 2023.
  - 3,000,000 Core-hours (XSEDE) - approved on Dec 15, 2021, for a period of 1 year starting from Jan 01, 2022.
- Update and maintain a database: Khazana
- Backup data generated by our group members
- Allocate computational resources among group members

## MENTORING EXPERIENCE

2020-present **Keara G Frawley**, *Grad student*.

**Research Topic:** Design of materials tolerant to spall failure at high strain rates.

**Key achievement:** Trained surrogate models to predict spall strengths of metals and alloys.

## ACADEMIC SERVICE

2016-2023 Served as a peer-reviewer for 20 articles, *Journal names include J. Chem. Phys., iScience, Digital Discovery, Int. J. Quantum Chem., J. Chem. Inf. Model, J. Mol. Liq., Macromolecules, Npj Comput. Mater., ACS omega, Patterns, ACS Appl. Nano Mater., Comput. Mater. Sci., J. Mater. Chem. C, Org. Electron*.

## TECHNICAL SKILLS

Programming language Python

Contribution to Software Development PCE predictor [[https://github.com/harikrishna-chem/opv\\_aem\\_2018](https://github.com/harikrishna-chem/opv_aem_2018)], Polymer structure predictor (PSP) [<https://github.com/Ramprasad-Group/PSP>], Polymer version of Computational Autonomy for Materials Discovery (CAMD)

*ab-initio*/MD Molpro, Orca, Gaussian, VASP, and LAMMPS

Machine learning Scikit-learn, Keras, and TensorFlow

Others OpenBabel, RDKit, GitHub, and Multiwfn

## AWARDS AND FELLOWSHIPS

- 4 Received the *first prize at the AMDD hackathon* organized by Toyota Research Institute, May 26-29, **2020**. Demonstrated how cheap experiments can be more valuable than fewer expensive ones.

- 3 Selected for a *Special international postdoc grant* by Nanjing university, Mar. **2017** - Feb. **2019**.
- 2 Qualified *National eligibility test (NET)*, **2011** in the subject of Chemical Sciences under UGC fellowship scheme - secured 0088/1065 rank.
- 1 Qualified *Graduate aptitude test in engineering (GATE)*, **2011** in the subject of Chemistry - All India rank - 1010.

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## PROFESSIONAL ASSOCIATIONS

- 2016-present Orissa Chemical Society - Life Member: LM/1067/16  
2021-2022 Materials Research Society - ID: 11129383  
2021-2022 American Chemical Society - ID: 32637228

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## TEACHING EXPERIENCE

- 07/15–12/15 **Teaching Assistantship**, IIT GUWAHATI, Assam, B.Tech. PH305.  
Computational Physics Lab
- 07/14–12/14 **Teaching Assistantship**, IIT GUWAHATI, Assam, B.Tech. CH101.  
Tutorial class on Physical Chemistry
- 07/13–12/13 **Teaching Assistantship**, IIT GUWAHATI, Assam, B.Tech. CH110.  
General Lab
- 07/12–12/12 **Teaching Assistantship**, IIT GUWAHATI, Assam, B.Tech. CH314.  
Chemical Technology Lab II

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## PERSONAL INFORMATION

- Nationality Indian  
Sex Male  
Languages English, Hindi, Odia  
Date of birth 31 Oct. 1989