

CV of Dr. Nilanjan Roy (He/Him/His)

Birth date: 04/03/1995 Nationality: Indian Unmarried ORCID: 0000-0002-0386-4950;
Departmental webpage: <https://chemistry.nits.ac.in/faculties/nilanjan-roy>; Google Scholar: [Nilanjan Roy](#)

EDUCATION

2017-2022: Ph.D. in Solid State Chemistry & Crystallography, IIT Kharagpur, India; Supervisor: Prof. Partha Pratim Jana
2015-2017: M.Sc. Chemistry, IIT Bombay, India; M.Sc. Thesis Supervisor: Prof. C. P. Rao. (CGPA: 8.4)
2012-2015: B.Sc. Honors in Chemistry with Physics and Mathematics Minor. (First Class)

CURRENT POSITION

Assistant Professor at the Department of Chemistry; National Institute of Technology Silchar, Assam, India.

PREVIOUS POSITIONS

2023-2025: Postdoctoral Research Associate at the Department of Chemical Engineering, Penn State University (USA)
with Prof. Robert M. Rioux

RESEARCH ACHIEVEMENTS

My research focuses on the structural chemistry of intermetallic compounds and the establishment of composition–structure–property relationships through the integration of solid-state synthesis, crystallography, electronic structure calculations, and heterogeneous catalysis. My work spans three interconnected research areas: (1) synthesis and crystal chemistry of complex intermetallic compounds; (2) understanding chemical bonding and structure–property relationships using diffraction techniques and density functional theory (DFT); and (3) development of intermetallic materials for catalysis and hydrogen-related energy applications. More recently, I have contributed to machine learning-assisted discovery of intermetallic compounds by integrating data-driven methods (*Inorg. Chem.* **2024**, 63, 13, 5972–5981) with crystallographic and electronic-structure descriptors, providing a foundation for the accelerated design of functional intermetallic materials.

- **Structural chemistry of complex intermetallic compounds.** My doctoral research addressed the long-standing crystallographic "coloring problem" in Pd- and Cd-rich intermetallics arising from the low X-ray scattering contrast between neighbouring elements. This work resulted in the discovery and structure determination of several intermetallic phases, including Laves phases and γ -brass derivatives (*Z. Anorg. Allg. Chem.* **2022**, 648, e202100354), expanding the understanding of atomic ordering, occupational disorder, and structural complexity in intermetallic systems. These studies established structure–property relationships relevant to heterogeneous catalysis and hydrogen storage and developed expertise in solid-state synthesis, single-crystal and powder X-ray diffraction, neutron diffraction, and advanced crystallographic (both X-ray and neutron) refinement.
- **Electronic structure and chemical bonding in intermetallics.** I combine crystallographic analysis with first-principles calculations to understand the electronic origin of structural stability and physical properties. Using DFT along with bonding analysis tools such as COHP, COBI, and density of states calculations implemented in VASP, Quantum ESPRESSO, and LOBSTER, I have investigated the role of heteroatomic interactions, vacancies (*Inorg. Chem.* **2021**, 60, 8, 5488–5496), and electronic structure (*Z. Anorg. Allg. Chem.* **2023**, 649, e202300127) in stabilizing complex intermetallic compounds. This integrated experimental–computational approach has enabled quantitative correlations between crystal structure, chemical bonding, and materials properties (*Inorg. Chem.* **2025**, 64, 4, 1798–1807).
- **Intermetallic catalysts for selective hydrogenation.** As a postdoctoral researcher at The Pennsylvania State University, I have expanded my research toward heterogeneous catalysis (*Chem. Sci.* **2025**, 16, 20, 8611–8636) by developing Pd-based intermetallic catalysts for selective hydrogenation reactions (*ACS Catal.* **2026**, 16, 3, 2881–2890). My current work at NIT Silchar integrates crystallography, surface science, and catalytic evaluation to understand the relationship between crystal structure and catalytic performance, aiming to the identification of catalytically relevant intermetallic phases.

So far, I have published 30 peer-reviewed research articles (additional manuscripts under review and in preparation) spanning solid-state chemistry, crystallography, electronic structure, hydrogen storage, and heterogeneous catalysis. My research combines experimental and computational approaches to advance the rational design of functional intermetallic materials for energy-related applications.

AWARDS

Merit Cum Means: 2012

IIT JAM: 2015, AIR 40

CSIR NET JRF: 2016, AIR 59

OPA postdoctoral award from Penn State: 2025

Humboldt Research Fellowship for Postdocs: 2026, Host: Prof. Guido Kickelbick, Saarland University, Germany.

MSCA-CZ and MSCA COFUND: 2026, Host: Dr. Václav Petříček and Dr. Michal Dušek, Institute of Physics of the Czech Academy of Sciences, FZU, Prague, Czech Republic.

Visiting Scientist at the Department of Structure Analysis, Institute of Physics of the Czech Academy of Sciences, FZU, Prague, Czech Republic: May-July, 2027. Host: Dr. Václav Petříček and Dr. Michal Dušek,

ORGANISATION OF WORKSHOP/CONFERENCES

March 2026 Coordinator of a Five day workshop on Advanced Analytical Techniques for Materials Characterization and Skill Development at the Department of Chemistry, NIT Silchar.

Feb 2019 Participated in organizing a Global Initiative of Academic Networks (GIAN) course (Convener: Prof. P. P. Jana) on *Structure solution, refinement and interpretation of difficult inorganic structures by JANA 2006*, Invitees: Dr. Lukáš Palatinus, Dr. Mariana Klementova (FZU, Prague).

MAJOR CONFERENCES/WORKSHOPS

- National workshop on powder X-ray diffraction (NWPXRD-2017) at Pondicherry University (Dec 2017).
- Winter School on “Synchrotron Techniques in Materials Science” at SBNBCBS Kolkata (25-31 Oct 2018).
- National Conference on Crystallography (NSC-46) NIMHANS Bangalore: poster presentation (27-29 June 2018)
- Modern Trends in Inorganic Chemistry (MTIC-2019), Dept. of Chemistry, IIT Guwahati, poster (Dec 11-14, 2019).
- Pittsburgh-Cleveland Catalysis Society meeting (2023, 2024); poster presentation.
- NAM-2023, North American Catalysis Society Meeting. Providence, RI, USA (18 -23 June, 2023), poster presentation.
- Gordon Research Conference on Solid State Chemistry, poster presentation (21- 26 July 2024).
- NAM-2025, North American Catalysis Society Meeting, Atlanta, GA, USA. (8-12 June 2025): Oral presentation. Selected for postdoctoral travel grant award from office of postdoctoral affairs, Penn State.

SOFTWARE & EXPERIMENTAL EXPERTISE

User of ChemDraw, Diamond 5.0, VESTA, GSAS, CrysAlisPro, JANA 2006/2020 (Structure solution and refinement of single crystal X-ray diffraction data, Rietveld refinement of powder XRD and Neutron powder diffraction data), VASP (The Vienna Ab initio Simulation Package), APEX III, Quantum Espresso, LOBSTER for chemical bonding analysis (cohpp.de), wxDragon, LabView (Catalytic reactor).

- High-temperature solid-state synthesis, the flux method for crystal Growth; Experienced in solving crystal structures from single crystal X-ray diffraction data. Instruments used: glovebox, vacuum tube sealing unit, optical microscope; Single Crystal XRD (structure solution and refinement), Powder XRD (Rietveld refinement), Neutron powder diffraction (Rietveld refinement), Synchrotron X-ray powder diffraction (Proposal Preparation, Rietveld refinement) SEM (Scanning Electron Microscopy) and EDS (Energy Dispersive X-ray Spectroscopy), Infrared, Raman, UV-Visible and Inductively Coupled Plasma - Optical Emission Spectrometry Spectroscopy.
- Bulk electronic structure Calculation, Chemical Bonding Analysis (Crystal Orbital Hamilton Population), Bader Charge Analysis, *Coloring Problem* in Intermetallic Compounds (DFT-based).
- Chemical reactor (lab. scale) building and handling; collecting and analyzing reactor data using LabVIEW (from post- doct. lab), Synthesis of single-site catalysts using strong electrostatic adsorption (SEA) method (from post-doctoral lab).

TRAINING AND MENTORING

Currently mentoring 1 Ph.D. and 2 M.Sc. candidates at NIT Silchar as PI.; Mentored 1 Ph.D. candidate at Penn State. Mentored 3 M.Sc. and 2 junior Ph.D. candidates at IIT Kharagpur.

REVIEWER ACTIVITY IN MAJOR INTERNATIONAL JOURNALS

Zeitschrift für anorganische und allgemeine Chemie (1); *Journal of Alloys and Compounds* (4); *Journal of Physical Chemistry C* (1), *Nano Select* (1). *Journal of Catalysis* (1).

INTERNATIONAL COLLABORATORS

1. Prof. Robert M. Rioux (Penn State), 2. Prof. Michael J. Janik (Penn State), 3. Prof. James M. Hodges (Penn State), 4. Dr. Václav Petříček (FZU, Prague), 5. Dr. Michal Dušek (FZU, Prague), 6. Prof. Guido Kickelbick & Dr. Oliver Janka (University of Saarlands, Germany), 7. Dr. David PORTEHAULT (CNRS, Paris). 8. Dr. Jean-Claude Crivello (CNRS, Paris).

TEACHING

Currently actively involved in teaching for the following courses at NIT Silchar: Engineering Chemistry & Applied Chemistry for B.Tech; Physical Methods in Analytical Chemistry for M.Sc 2nd year & PhD.; and Inorganic and Physical Chemistry for M.Sc 1st year.

FULL PUBLICATION LIST TILL JULY 2026

(A) Review article: Publications with peer review process:

- 1) **Roy, N.**,[#] MacIntosh, K.,[#] Eid, M., Canning, G., & Rioux, R. M.* (2025). The structural chemistry of intermetallic compounds enables active site design in heterogeneous catalysis. *Chemical Science*. 2025, 16, 8611-8636.

(B) Further Publications: Publications with peer review process, arranged yearwise:

- 1) **Roy, N.**,^{*} Nag, J.; Corrêa, C. A.; Li, J.; Petříček, V.; Dušek, M.; Proffen, T.; Janik, M. J.; Rioux, R. M. (2026) CoSn-type $\text{Ni}_3\text{In}_{3-x}\text{Sb}_x$ ($x = 0-0.5$): Site-Selective Substitution, Electronic Structure, Chemical Bonding and Structural Transformation. *Manuscript just accepted in Inorganic Chemistry*.
- 2) Eid, M., Li, J., **Roy, N.**, MacIntosh, K., Rioux, R. M., & Janik, M. J. (2026). Substitution of Pd with Cu and Ag in InPd_3 intermetallics enhances net alkene selectivity in competitive acetylene hydrogenation. *Journal of Catalysis*, 462, 117083.
- 3) **Roy, N.**, Kuila, S. K.; Li, J.; Eid, M.; MacIntosh, K.; Pramanik, P.; Proffen, T.; Janik, M. J.*; Jana, P. P.*; Rioux, R. M.*. (2025) Solving 'Coloring Problem' in TiAl_3 -type $\text{InPd}_{3-x}\text{Ag}_x$ ($x = 0-1$) Intermetallic Compounds by Calculation of Phase Diagrams Modeling and Diffraction Experiments, *Inorganic Chemistry* 64 (48), 23535-23545.
- 4) Eid, M., **Roy, N.**,[#] Li, J. [#], MacIntosh, K., [#] Janik, M. J.,* Rioux, R. M.* (2026) Facet Preferencing by Chemical Substitution Controls Semi-Hydrogenation Selectivity in Ternary Pyrite-Type Intermetallic Compounds *ACS Catalysis*, 16 (3), 2881–2890.
- 5) Li, J., Gong, R., **Roy, N.**, Liu, Z. K., & Janik, M. J.* (2025). InPd_3 and InPd_2Cu Intermetallic Catalysts for Selective Hydrogenation Catalysis. *Industrial & Engineering Chemistry Research*, 64(12), 6354-6363.
- 6) Kuila, S. K., **Roy, N.**,[#] Pramanik,[#] P., Buxi, K., Bera, A. K., & Jana, P. P.* (2025). Unprecedented Site Preference of Sn in the Structure of CoSn-Type $\text{NiIn}_{1-x}\text{Sn}_x$ ($x < 0.7$). *Inorganic Chemistry*. 64(4), 1798–1807.
- 7) **Roy, N.**,^{*} Dutta, A., & Buxi, K. (2024). One electron is enough: A chemical bonding approach on the hydrogen induced structural transformation in MPd_3 (M= Mg, In, Tl) intermetallic compounds. *Journal of Solid State Chemistry*, 338, 124893
- 8) **Roy, N.*** (2024). A Fundamental Perspective on the Selective Zn Substitution in Ternary Ordered Intermetallic Compound $\text{Cu}_6\text{Zn}_2\text{Sb}_2$. *Zeitschrift für anorganische und allgemeine Chemie*, 650(13-14), e202400030.
- 9) Sikdar, R., **Roy, N.**, Selvaratnam, B., Mishra, V., Mumbaraddi, D., Mondal, A., Buxi, K., Jana, P.P. & Mar, A.* (2024). Ahead by a century: Discovery of Laves phases assisted by machine learning. *Inorganic Chemistry*, 63(13), 5972-5981.
- 10) **Roy, N.*** (2024). The search for optimum host-guest interactions: Atomic hydrogen storage properties of the

novel ternary ordered intermetallic compound Cu₃ZnSb: A DFT study. *International Journal of Hydrogen Energy*, 50, 854-864.

- 11) **Roy, N.,*** & Giri, S. (2024). Influence of the Homoatomic and Multicenter Bonding on the Formation of CsCl-type RhCd. *Zeitschrift für anorganische und allgemeine Chemie*, 650(5-6), e202300232.
- 12) **Roy, N.*** (2023). Atomic hydrogen storage in ternary InPd₂Cu–electronic structure and chemical bonding approach: a DFT study. *International Journal of Hydrogen Energy*, 48(91), 35639-35649.
- 13) **Roy, N.*** (2023). A Theoretical Study on the Unique Site Preference and Atomic Ordering of Hexagonal CoSn-type Ternary Intermetallic Compound Co₃Ge₂Sn. *Zeitschrift für anorganische und allgemeine Chemie*, 649(22), e202300127.
- 14) **Roy, N.*** (2023). Understanding formation of the InPd₃ polymorphs: a DFT study. *Zeitschrift für Naturforschung B*, 78(6), 355-361. (Editor's choice for cover art)
- 15) Kuila, S.K.,# Harshit,# **Roy, N.**, Ghanta, S., Pan, R., Buxi, K., Pramanik, P., Bera, A.K., Saha, B., Yusuf, S.M., Roy, A., Petříček, V., Jana, P. P.* (2023). Ni₃InSb: Synthesis, Crystal Structure, Electronic Structure, and Magnetic Properties. *Inorganic Chemistry*, 62(19), 7304-7314.
- 16) **Roy, N.**, Kuila, S. K., Harshit, Pramanik, P., & Jana, P. P.* (2022). Selective chemical substitution of Cu in the structure of TiAl₃ type InPd₃: experimental and theoretical studies. *European Journal of Inorganic Chemistry*, 2022(26), e202200309.
- 17) **Roy, N.**, Kuila, S. K., Mondal, A., Sikdar, R., Ghanta, S., Wang, F., & Jana, P. P.* (2022). Crystal structure, electronic structure and phase stability of the Cu_{2-x}M_xCd (M= Zn, Ga, Ge, Sn) pseudo-binary Laves phases: effect of valence electron concentration. *Journal of Solid State Chemistry*, 313, 123283.
- 18) **Roy, N.**, Harshit, Mondal, A., Wang, F., & Jana, P. P.* (2022). Structural and Theoretical Investigations on the Unique Coloring Scheme of the γ -Brass Type Phase: Cu_{5+ δ} Cd_{8- δ} ($-1.0 \leq \delta \leq 0.1$). *Zeitschrift für anorganische und allgemeine Chemie*, 648(15), e202100354.
- 19) **Roy, N.**,# Harshit,# Jana, P. P.* (2022). Hydrogen storage properties of ternary ordered cubic Laves phase Cu₃Cd₂In: Electronic structure and bonding approach. *Journal of Solid State Chemistry*, 312, 123223.
- 20) **Roy, N.**, Koley, B., Harshit, & Jana, P. P.* (2022). Formation and stability of Rh₂Cd₅ and its structural correlation with RhCd and Rh₃Cd_{5- δ} ($\delta \sim 0.56$). *Zeitschrift für Kristallographie-Crystalline Materials*, 237(6-7), 233-238.
- 21) **Roy, N.**, Kumari, S., Harshit, Jana, P. P., & Deshpande, P. A. (2021). Hydrogen storage properties of hexagonal C14 Laves phase Cu₂Cd: A DFT study. *Journal of Solid State Chemistry*, 304, 122560.
- 22) **Roy, N.**, Giri, S., Harshit, & Jana, P. P.* (2021). Site preference and atomic ordering in the ternary Rh₅Ga₂As: first-principles calculations. *Zeitschrift für Kristallographie-Crystalline Materials*, 236(5-7), 147-154.
- 23) **Roy, N.**, Kumari, S., Sikdar, R., Sharma, A., Harshit, Ghanta, S., Sharma, S., Deshpande, P.A. and Jana, P.P.,* (2021). Synthesis, Crystal Structure, Electronic Structure, and Catalytic Properties of Ni₃GaSb. *European Journal of Inorganic Chemistry*, 2021(14), 1410-1418.
- 24) **Roy, N.**,# Koley, B.,# Harshit, Mallick, S., Simonov, A., & Jana, P. P.* (2021). A Vacancy-Driven Intermetallic Phase: Rh₃Cd_{5- δ} ($\delta \sim 0.56$). *Inorganic Chemistry*, 60(8), 5488-5496.
- 25) **Roy, N.**,# Harshit,# Chakrabarty, A., & Jana, P. P.* (2021). Site preference, atomic ordering, electronic structure

and chemical bonding of A_3Pd_5 ($A = Mg, Al, Ga$): First principles study. *Solid State Sciences*, 113, 106544.

26) **Roy, N.**, Chakrabarty, A., Koley, B., Saha-Dasgupta, T., & Jana, P. P.* (2020). Site preference and atomic ordering in the structure of In_3Pd_5 : A theoretical study. *Journal of Solid State Chemistry*, 290, 121567.

27) Ghanta, S., **Roy, N.**, & Jana, P. P.* (2020). Crystal structures of two very similar $2 \times 2 \times 2$ superstructures of γ -brass-related phases in ternary Ir–Cd–Cu system. *Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials*, 76(1), 47-55.

(C) Contribution to other research field (Soil Science): Publications with peer review process:

1) Barrow, N. J., Sen, A., **Roy, N.**, & Debnath, A. (2021). The soil phosphate fractionation fallacy. *Plant and Soil*, 459, 1-11.

(D) Publications without peer review process: Conference presentations:

1) **Roy, N.**, Eid, M., Li, J., MacIntosh, K., Janik, M., & Rioux, R.* (2025, June) Selective Chemical Substitution of Pd-Rich Intermetallic Catalysts Enhances Net Ethylene Selectivity during Competitive Acetylene Hydrogenation. In *The 29th North American Catalysis Society Meeting*. AIChE. (as a presenting/lead author)

2) Eid, M., **Roy, N.**, MacIntosh, K., Janik, M., & Rioux, R.* (2025, June). Facet Preferencing by Chemical Substitution Controls Semi-Hydrogenation Selectivity in Ternary Pyrite-Type Intermetallics. In *The 29th North American Catalysis Society Meeting*. AIChE.

3) Li, J., Eid, M., **Roy, N.**, Rioux, R., & Janik, M.* (2024, October). Structure, Stability, and Selective Hydrogenation Catalysis Using Ternary Intermetallics. In *2024 AIChE Annual Meeting*. AIChE.

(E) Publications in pre-print services (open science): without peer review process:

1) **Roy, N.*** & Kuila, S. K. (2023). Selective Chemical Substitution in Intermetallic Compounds: DFT Study of Two Representative Cases: $Cu_5Zn_3Sb_2$ and $InPd_2Cu$. *chemrxiv.org*

(F) Manuscripts under preparation: to be submitted for peer review by 2026:

1) **Roy, N.***, Nag, J.P., Janik, M., & Rioux, R.* A Quantitative Approach on the Chemical Bonding of α -Gallium: Combined DFT and Scanning Tunneling Electron Microscopy Study. Target journal: *Chemistry: A European Journal*.

2) **Roy, N.***; Eid, M.; Janik, M. J.; Rioux, R. M. Chemical and Electronic Origins of Limited Au Solubility in Pyrite-Type $PdSb_2$; Target journal: *Inorganic Chemistry*.

3) **Roy, N.***; Kuila, S. K.; Janik, M. J.; Jana, P. P.; Rioux, R. M. Valence Electron Concentration Dictates the Structural Transformation in Pseudo-Binary $Cu_{2-x}Sb_xCd$ ($x = 0-0.3$) Laves Phases. Target Journal: *Chemistry of Materials*.

NOTE: *Corresponding Author; #Equal Contribution

Declaration: I hereby declare that the information provided above is true, complete, and accurate to the best of my knowledge and belief.

NIT Silchar
26/07/2026

Nilanjan Roy