

Curriculum Vitae:

Name: Apurba Kumar Patra

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Benachiti, Durgapur-713 213

Academic Qualification:

- ❖ MSc (Inorganic Chemistry specialization)
Burdwan University (1990-1992), WB, India
- ❖ PhD (1993-1999 under supervision of Prof. R. Mukherjee)
Indian Institute of Technology (IIT) Kanpur
Kanpur-208 016, UP, India

Post-Doctoral Research:

- ❖ Dept. of Chemistry, University of Georgia, Athens, USA. (November 1999-October 2000 in Lab of Prof. Charles R. Kotal)
- ❖ Dept. of Chemistry, University of Louisville, Kentucky, USA. (November 2000- October 2001 in Lab of Prof. Craig A. Grapperhaus)
- ❖ Dept. of Chemistry & Biochemistry, University of California, Santa Cruz, USA. (November 2001- October 2004 in Lab of Prof. Pradip K. Mascharak)
- ❖ Alexander von Humboldt Fellow, Max-Planck-Institute für Bioanorganische Chemie, Mülheim an der Ruhr, Germany. (April 2005- March 2006 in Lab of Prof. Karl Wieghardt)

Positions at NIT Durgapur:

- ❖ Assistant Professor: 2006-2009
- ❖ Associate Professor: 2009-2018
- ❖ Associate Professor & Head of the Department: 2013-2015
- ❖ Professor: Since 2018-

Research Interests: Our research focused to understand the intrinsic properties of metal ions in certain ligand donor environments, mimicking biological metal active sites. We synthesize the targeted complexes of mainly Cu and Ni ions in N, S donor coordination environment and study their electronic properties by means of various spectroscopic methods including X-ray structure determination. The spectroscopic measurements include: FT-IR, ¹H NMR, UV-Vis, UV-Vis-NIR, cyclic voltammetry, EPR, fluorescence, ESI Mass and

others if required. Spectro-electrochemistry plays a vital role to study (a) the nature of redox reactions and (b) the stability of metal oxidation states involved to show the reactivity with small molecules.

We have successfully contributed to the Modelling work of biological (a) Copper active sites of few copper containing enzymes such as: Copper Nitrite Reductase (**CuNiR**), Cu_M site of Hydroxylases (i.e. Dopamine-β-monooxygenase), Copper-Zinc Superoxide Dismutase (**CuZn-SOD**), Cu_A & Cu_Z sites (of Cytochrome-c-Oxidase, CcO, and Nitrous Oxide Reductase, N₂OR) and (b) Nickel active sites of enzymes such as Ni containing Superoxide Dismutase (Ni-SOD), the Ni_P Site of Carbonmonoxide Dehydrogenase/Acetyl-Coenzyme A Synthase (**CODH/ACS**) and the key step of the catalytic cycle of Methyl-Coenzyme M Reductase (**MCR**). We usually investigate the reactivity of small molecules such as Nitric Oxide (NO), Carbon Monoxide (CO), Dioxygen (O₂), Superoxide Radical Anions (O₂⁻) with the synthesized model complexes. These reactivity studies are highly important, help to elucidate the mechanism of catalytic action and the role of metal active sites of the enzymes in biology.

List of Publications

S. No.	Author(s)	Title	Name of Journal	Vol	Page	Year
43	S. Kumar, S. Mishra, A. Das, K. Mahiya, S. Laha, M. Maji, A. K. Patra*	Analogues Copper Nanoclusters (Cu _{16/17}) with Two Electron Superatomic and Mixed Valence Copper(II)/Copper(I) and Copper(I)/Copper(0) Characters.	Nanoscale	16	DOI: 10.1039/D4NR03578J	2024
42	S. Mishra, S. Kumar, A. Bhandari, A. Das, P. Mondal, G. Hundal, M. M. Olmstead, A. K. Patra*	Reactivity of Nitric Oxide and Nitrosonium Ion with Copper (II/I) Schiff Base Complexes: Mechanistic Aspects of Imine C=N Bond Cleavage and Oxidation of Pyridine-2-aldehyde to Pyridine-2-carboxylic Acid.	Inorg. Chem	61	6421-6437	2022
41	S. Mishra, A. Bhandari, D. Singh, R. Gupta, M. M. Olmstead, A. K. Patra*	Bis(μ-thiolato)-dicopper Containing Fully Spin Delocalized Mixed Valence Copper-sulfur Clusters and Their Electronic Structural Properties with Relevance to the Cu _A Site.	Inorg. Chem	60	5779-5790	2021
40	A. Bhandari, S. Mishra, R. C. Maji, A. Kumar, M. M. Olmstead, A. K. Patra*	Ni(II)-Mediated Reversible Thiolate/Disulfide Conversion as a Mimic for a key Step of the Catalytic Cycle of Methyl-Coenzyme M Reductase.	Angew. Chem. Int. Ed.	59	9177-9185	2020
39	K. K. Pobi, B. Mondal, S. Nayek,	Efficient removal of Hg ²⁺ , Cd ²⁺ and Pb ²⁺ from	Water Science and Technology	79	1092-1102	2019

	A. K. Patra, R. Saha	aqueous solution and mixed industrial wastewater using designed chelating ligand, 2-pyridyl-N-(2-methylthiophenyl)methyleneimine (PMTPM).				
38	A. Bhandari, R. C. Maji, S. Mishra, A. Kumar, S. K. Barman, P. P. Das, M. M. Olmstead, A. K. Patra*	Model Complexes for the Ni _p Site of Acetyl Coenzyme A Synthase/Carbon Monoxide (CO) Dehydrogenase: Structure, Electrochemistry, and CO Reactivity.	Inorg. Chem	57	13713-13727	2018
37	R. C. Maji, S. Mishra, A. Bhandari, R. Singh, M. M. Olmstead, A. K. Patra*	A Cu ^{II} -nitrite That Exhibits Change of Nitrite Binding Mode and Formation of Cu ^{II} -Nitrosyl Prior to NO Evolution	Inorg. Chem	57	1550-1561	2018
36	R. C. Maji, P. P. Das, A. Bhandari, S. Mishra, M. Maji, ^a K. B. Ghiassi, M. M. Olmstead, A. K. Patra*	Mixed Valence Copper-sulfur Clusters of Highest Nuclearity: A Cu ₈ Wheel and a Cu ₁₆ Nanoball	Chem. Commun	53	3334-3337	2017
35	Ram Chandra Maji, Partha Pratim Das, Saikat Mishra, Anirban Bhandari, Milan Maji, Apurba K. Patra*	Electron Transfer Mechanism of Catalytic Superoxide Dismutation <i>via</i> Cu(II/I) Complexes: Evidence of Cupric-superoxo/hydroperoxo Species	Dalton Transaction	45	11898-11910	2016
34	Alok Dutta, Sourav Kr. Saha, Priyabrata Banerjee, Apurba K. Patra , Dipankar Sukul.	Evaluating Corrosion Inhibition Property of some Schiff Bases for Mild Steel in 1 M HCl: competitive effect of the heteroatom and stereochemical conformation of the molecule	RSC Adv.	6	74833-74844	2016
33	Ram Chandra Maji, Anirban Bhandari, Ravindra Singh, Suprakash Roy, Sudip K. Chatterjee, F. L. Bowles, K. B. Ghiassi, Milan Maji, Marilyn M.	Copper Coordinated Ligand Thioether-S and NO ₂ ⁻ Oxidation: Relevance to Cu _M Site of Hydroxylases	Dalton Transaction	44	17587-17599	2015

	Olmstead, Apurba K. Patra*					
32	Sudip K. Chatterjee, Ram Chandra Maji, Suman K. Barman, Marilyn M. Olmstead, Apurba K. Patra*	Hexacoordinate Ni(II)/Ni(III) Complexes that Mimic the Catalytic Cycle of Nickel Superoxide Dismutase	<i>Angew. Chem. Int. Ed.</i>	53	10184-189	2014
31	Ram Chandra Maji, Suman Kumar Barman, Suprakash Roy, Sudip K. Chatterjee, Faye L. Bowles, Marilyn M. Olmstead, Apurba K. Patra*	Copper Complexes Relevant to the Catalytic Cycle of Copper Nitrite Reductase: Electrochemical Detection of NO(g) Evolution and Flipping of NO ₂ Binding Mode upon Cu ^{II} → Cu ^I Reduction	<i>Inorg. Chem.</i>	52	11084-095	2013
30	Sudip K. Chatterjee, Suprakash Roy, Suman Kumar Barman, Ram Chandra Maji, Marilyn M. Olmstead, Apurba K. Patra*	Shuttling of Nickel Oxidation States in N ₄ S ₂ Coordination Geometry vs. Donor Strength of Tridentate N ₂ S Donor Ligands	<i>Inorg. Chem.</i>	51	7625-35	2012
29	Suprakash Roy, Saleem Javed, Marilyn M. Olmstead and Apurba K. Patra*	First Structural Example of a Metal Un-coordinated Mesoionic Imidazo[1,5-a]pyridine and its Precursor Intermediate Copper Complex: An Insight to the Catalytic Cycle	<i>Dalton Trans.</i>	40	12866-876	2011
28	Suprakash Roy, Partha Mitra, Apurba K. Patra*	Cu(II) complexes with square pyramidal (N ₂ S)CuCl ₂ chromophore: Jahn-Teller distortion and subsequent effect on spectral and structural properties	<i>Inorg. Chim. Acta</i>	370	247-253	2011
27	Michael J. Rose, Apurba K. Patra , Marilyn M. Olmstead, Pradip K. Mascharak	Structural and spectroscopic evidence for linkage isomerism of bound nitrite in a {Fe-NO} ⁶ nitrosyl derived from a tetradentate dicarboxamide ligand: More parallels between heme and non-heme systems	<i>Inorg. Chim. Acta</i>	363	2715-2719 (Spl. Issue for Prof. Animesh Chakravorty Birth Day)	2010

26	Haritosh Mishra, Apurba K. Patra , Rabindranath Mukherjee	Relative stability of half-sandwiched η^6 -benzene Ru^{II} complexes of tridentate (2-pyridyl) alkylamine ligands of varying chelate ring size: Nucleophilic addition of hydride ion onto the benzene ring	<i>Inorg. Chim. Acta</i>	362	483-490	2009
25	Michael J. Rose, Apurba K. Patra , Eric A. Alcid, Marilyn M. Olmstead and Pradip K. Mascharak	Ruthenium Nitrosyls Derived from Polypyridine Ligands with Carboxamide or Imine Nitrogen Donor(s): Isoelectronic Complexes with Different NO Photolability	<i>Inorg. Chem.</i>	46	2328-2338	2007
24	P. K. Mascharak, A. K. Patra, R. K. Afshar, A. A. Eroy-Reveles	Is heme Chemistry distinct from non-heme chemistry?	<i>J. Porphyrin Phthalocynin</i>	10	341	2006
23	Melanie Madhani, Apurba K. Patra , Thomas W. Miller, Aura A. Eroy-Reveles, Adrian Hobbs, Jon M. Fukuto, and Pradip K. Mascharak	Biological Activity of Designed Photolabile Metal Nitrosyls: Light Dependent Activation of Soluble Guanylate Cyclase and Vasorelaxant Properties in Rat Aorta	<i>J. Med. Chem.</i>	49	7325-7330	2006
22	Apurba K. Patra , Eckhardt Bill, Eberhard Bothe, Krysztof Chlopek, Frank Neese, Thomas Weyhermüller, Keira Stobie, Michael D. Ward, Jon A. McCleverty and Karl Wiegardt	The Electronic Structure of Mononuclear Bis(1,2-diaryl-1,2-ethylenedithiolato)iron Complexes Containing a Fifth Cyanide or Phosphite Ligand: A Combined Experimental and Computational Study	<i>Inorg. Chem.</i>	45	7877-7890	2006
21	Apurba K. Patra , Eckhardt Bill, Thomas Weyhermüller, Keira Stobie, Zoe Bell, Michael D. Ward, Jon A. McCleverty and Karl Wiegardt	Dinuclear Bis(1,2-diaryl-1,2-ethylenedithiolato)iron Complexes: $[Fe_2^{III}(L_4)]^n$ ($n = 2-, 1-, 0, 1+$)	<i>Inorg. Chem.</i>	45	6541-6548	2006
20	Raman K. Afshar, Apurba K. Patra , Eckhardt Bill, Marilyn M. Olmstead, and Pradip K. Mascharak	Synthesis, Structure, and Properties of an Fe(II) Carbonyl $[(PaPy_3)Fe(CO)](ClO_4)$: Insight into the Reactivity of Fe(II)-CO and Fe(II)-NO Moieties	<i>Inorg. Chem.</i>	45	3774-3781	2006

		in Non-Heme Iron Chelates of N-donor Ligands				
19	Raman K. Afshar, <u>Apurba K. Patra</u> , and Pradip K. Mascharak	Light-induced Inhibition of Papain by a {Mn-NO} ⁶ Nitrosyl: Identification of Papain-SNO Adduct by Mass Spectrometry	<i>J. Inorg. Biochem.</i>	99	1458-1464	2005
18	<u>Apurba K. Patra</u> , Michael J. Rose, Marilyn M. Olmstead, and Pradip K. Mascharak	Reactions of Nitric Oxide with a Low-spin Fe(III) Center Ligated to a Tetradentate Dicarboxamide N ₄ Ligand: Parallels between Heme and Non-heme Systems	<i>J. Am. Chem. Soc.</i>	126	4780-4781	2004
17	Raman K. Afshar, <u>Apurba K. Patra</u> , Marilyn M. Olmstead, and Pradip K. Mascharak	Syntheses, Structures and Reactivities of {Fe-NO} ⁶ Nitrosyls Derived from Polypyridine-Carboxamide Ligands: Photoactive NO Donors and Reagents for S-nitrosylation of Alkyl Thiols	<i>Inorg. Chem.</i>	43	5736-5743	2004
16	<u>Apurba K. Patra</u> , Michael J. Rose, Karen Murphy, Marilyn M. Olmstead, and Pradip K. Mascharak	Photolabile Ruthenium Nitrosyls with Planar Dicarboxamide Tetradentate N ₄ Ligands: Effect of in-plane and Axial Ligand Strength on NO Release	<i>Inorg. Chem.</i>	43	4487-4495	2004
15	<u>Apurba K. Patra</u> , and Pradip K. Mascharak	Sensing and Fixation of NO ₂ /N ₂ O ₄ by Calix[4]Arenes	<i>Chemtrac Inorg. Chem.</i>	17	183-188	2004
14	<u>Apurba K. Patra</u> , Raman K. Afshar, John M. Rowland, Marilyn M. Olmstead, and Pradip K. Mascharak	Thermally-Induced Stoichiometric and Catalytic O Atom Transfer by a Non-heme Iron(III)-Nitro Complex: First Example of Reversible {Fe-NO} ⁷ ↔ Fe ^{III} -NO ₂ Transformation in Presence of Dioxygen	<i>Angew. Chem. Int. Ed.</i>	42	4517-4521	2003
13	<u>Apurba K. Patra</u> and Pradip K. Mascharak	A Ruthenium Nitrosyl That Rapidly Delivers NO to Proteins in Aqueous Solution Upon Short Exposure to UV Light	<i>Inorg. Chem.</i>	42	7363-7365	2003
12	<u>Apurba K. Patra</u> , John M. Rowland,	Iron-nitrosyls of a Pentadentate Ligand	<i>Inorg. Chem.</i>	42	6812-6823	2003

	Dana S. Marlin, Eckhardt Bill, Marilyn M. Olmstead, and Pradip K. Mascharak	Containing a Single Carboxamide Group: Syntheses, Structures, Electronic properties, and Photolability of NO				
11	Craig A. Grapperhaus, Ming Li, <u>Apurba K. Patra</u> , Selma Poturovic, Pawel M. Kozlowski, Marek Z. Zgierski, and Mark S. Mashuta	Synthesis and Characterization of N ₂ S ₃ X-Fe Models of Iron-Containing Nitrile Hydratase	<i>Inorg. Chem.</i>	42	4382-4388	2003
10	<u>Apurba K. Patra</u> , Raman Afshar, Marilyn M. Olmstead, and Pradip K. Mascharak	The First Non-Heme Iron(III) Complex with a Ligated Carboxamido Group That Exhibits Photolability of a Bound NO Ligand	<i>Angew. Chem. Int. Ed.</i>	41	2512-2515	2002
9	<u>Apurba K. Patra</u> , Marilyn M. Olmstead, and Pradip K. Mascharak	Spontaneous Reduction of a Low-spin Fe(III) Complex of a Neutral Pentadentate N ₅ Schiff-base Ligand to the Corresponding Fe(II) Species in Acetonitrile	<i>Inorg. Chem.</i>	41	5403-5409	2002
8	Craig A. Grapperhaus, <u>Apurba K. Patra</u> , and Mark S. Mashuta	First {Fe-NO} ⁶ Complex with an N ₂ S ₃ Fe-NO Core as a Model of NO-Inactivated Iron-Containing Nitrile Hydratase. Are Thiolates and Thioethers Equivalent Donors in Low-Spin Iron Complexes?	<i>Inorg. Chem.</i>	41	1039-1041	2002
7	<u>Apurba K. Patra</u> and Pradip K. Mascharak	C-H Bond Activation by a Ferric Methoxide Complex: Modeling the Rate-Determining Step in the Mechanism of Lipoxygenase	<i>Chemtrac Inorg. Chem.</i>	15	282-288	2002
6	Craig A. Grapperhaus, <u>Apurba K. Patra</u> , Selma Poturovic, and Mark S. Mashuta	Synthetic Models of Nitrile Hydratase	<i>J. Inorg. Biochem.,</i>	86	240	2001
5	<u>Apurba Kumar Patra</u> , Manabendra Ray, and Rabindranath Mukherjee	Magneto-structural Studies of Monohydroxo-bridged Dicopper(II) Complexes M[Cu ₂ L ₂ (OH)]·2H ₂ O (M = Na ⁺ (1) and K ⁺ (2); H ₂ L = 2,6-	<i>Polyhedron</i>	19	1423-1428	2000

		bis[N-(phenyl)carbamoyl]pyridine. Effect of Cu-OH-Cu Bridge Angle on Antiferromagnetic Coupling.				
4	<u>Apurba Kumar Patra</u> , Manabendra Ray, Rabindranath Mukherjee and	Synthesis and Characterization of Pyridine Amide Cation Radical Complexes of Iron: Stabilization Due to Coordination with Low-Spin Iron(III) Center	<i>Inorg. Chem.</i>	39	652-657	2000
3	<u>Apurba Kumar Patra</u> and Rabindranath Mukherjee	Synthesis and Properties of a Monomeric and a μ -Oxo Bridged Dimeric Iron(III) Complex with Tetradentate Pyridine Amide in-plane Ligand. X-ray Structure of [Fe(bpc)Cl(DMF)] ($H_2bpc = 4,5$ -dichloro-1,2-bis(pyridine-2-carboxamido)benzene)	<i>Polyhedron</i>	18	1317-1322	1999
2	<u>Apurba Kumar Patra</u> , Manabendra Ray, Rabindranath Mukherjee and	Synthesis, Crystal Structure and Properties of Trigonal Bipyramidal $[M(L^5)_2(H_2O)] \cdot H_2O$ complexes [M = cobalt(II) ($S = 3/2$) and copper(II) ($S = 1/2$); $HL^5 = N$ -2-chloro-6-methylphenyl-pyridine-2-carboxamide]	<i>J. Chem. Soc., Dalton Trans</i>	-	2461-2466	1999
1	<u>Apurba Kumar Patra</u> and Rabindranath Mukherjee	Bivalent, Trivalent, and Tetravalent Nickel Complexes with a Common Tridentate Deprotonated Pyridine Bis-Amide Ligand. Molecular Structures of Nickel(II) and Nickel(IV) and Redox Activity	<i>Inorg. Chem.</i>	38	1388-1393	1999

News Highlights in Chemical & Engineering News:

1	Light makes iron complex let go of NO	Chemical and Eng. News	80 (No. 28)	30	2002
2	Iron-nitro catalyst transfers oxygen	Chemical and Eng. News	81 (No. 40)	24	2003

Papers published in Conferences/Symposium:

S.No.	Title of paper	Co-author(s), if any	Name of the Conference	Date & year
1	Modeling Oxygenated Cysteine Thiolates with a Thiolate/Thioether Donor Set. A Structural and Spectroscopic Model of NO-inactivated Iron-containing Nitrile Hydratase	C. A. Grapperhaus, A. K. Patra , M. Li, S. Poturovic, M. S. Mashuta	<i>The American Chemical Society</i>	224: 049-Inorg Part I Aug 13-18 2002
2	Synthesis of a Tetradentate Histidine-phenol Crosslink that mimics the Active Site of Cytochrome c Oxidase to Study the Reduction of Dioxygen to Water	Landavery, Y. R., White, K. N., Praveen, N., Konopelski, J. P., Sen, I., Patra, A. K. , Olof, E.	<i>The American Chemical Society</i>	229: 049-Inorg Part I March 13-17, 2005
3	Ruthenium Nitrosyls Derived from Polypyridine N5 Carboxamide or N5 Schiff Base Ligands: Comparison of Stability and NO Photolability in Aqueous Solution	Rose, M. J., Patra, A. K. , Mascharak, P. K.	<i>The American Chemical Society</i>	229: 049-Inorg Part I March 13-17, 2005 .
4	A Series of Di-iron Complexes of Formulae [FeIII ₂ (L) ₄] _n (n = 2-, 1-, 0, 1+) of Redox Non-innocent 1,2-diaryl-1,2-ethylenedithiolate Ligands and Their Reactivity.	Patra, A. K. , Bill, E., Weyhermüller, T., Stbie, K., Bell, Z., Ward, M., McCleverty, J. A., Wieghardt, K.	<i>Conference on Inorganic Scientific Perspective</i>	December 21, 2008
5	Copper Ion Mediated Synthesis of Mesoionic Heterocycle and Its Antibacterial Studies.	Roy, S., Mitra, P., Patra, A. K.	<i>International Symposium on Frontiers in Inorganic Chemistry</i>	December 11-13, 2010
6	Copper Ion Catalyzed Mild Synthesis of Mesoionic Imidazo[1,5-a]Pyridines and Their Biological Reactivities: Implicit Information to the Catalytic Cycle	Roy, S., Chatterjee, S. K., Chandra, G., Maji, M., Patra, A. K.	<i>Symposium on Modern Trends in Inorganic Chemistry-XIV</i>	Dec 10-13, 2011
7	Functional Modelling of Copper Nitrite Reductase	Maji, R. C., Chatterjee, S. K., Maji, M., Barman, S. K., Olmstead, M. M., Patra, A. K.	<i>International Symposium on Modern Trends in Inorganic Chemistry-XV</i>	Dec 13-16, 2013

8	Effect of Ligand Donor Strength towards Stabilization of Various Oxidation State of Ni in N, S Coordinating Environment.	Chatterjee, S. K., Roy, S., Maji, R. C., Patra, A. K.	National Conference on <i>Recent Developments in Chemistry</i>	October, 03-05, 2013
9	Functional modelling of Type-2 Copper Site of Copper Nitrite Reductases	Maji, R. C., Chatterjee, S. K., patra, A. K.	National Conference on <i>Recent Developments in Chemistry</i>	October, 03-05, 2013
10	Chemical Modification of Polysaccharides from Waste Biomass and their Antioxidant	Utpal Adhikari, Apurba K. Patra	National Symposium on Recent Trends and Perspectives in Chemistry 2015	January 23-24, 2015
11	Substitution Reaction of Thio-ether and Thiols on Dinuclear Pd(II) Complex: Kinetic, Mechanism, Bioactivity and Docking	Apurba K. Patra , T. K. Saha, Sankar Ch. Moi	National Symposium on Recent Trends and Perspectives in Chemistry 2015	January 23-24, 2015
12	Ligand Donor Type Dictates The Cu ^{II/I} Mediated Thioether-S Oxidation: Insight to the Cu _M Site of Hydroxylases	R. C. Maji, A. Bhandari, S. C. Moi, M. Maji, Apurba K. Patra	International Symposium on <i>Modern Trends in Inorganic Chemistry-XVI</i>	December 03-05, 2015

Research Project / Sponsored project/ Consultancy activities:

Sponsoring Agency	Title of the Project	Period	Amount	Status(Completed/ongoing)
DST-SERC	Synthetic Modeling of Copper-Proteins Active Site	25.07.2008-24.07.2011	23,93,000	Completed
DST-SERB	Nickel Complexes Supported by N,S-Donor Ligands: Relevance to the Active Site of Acetyl CoA Synthase	01.11. 2015-31.10.2018	65,00,000	Completed

Professional Recognition/Award/Prize/Certificate, Fellowship received:

S. No.	Name of award	Awarding agency	Year
1	Alexander von Humboldt Fellowship	AvH Foundation, Germany	2005