

# Subhajyoti Chaudhuri

📍 Department of Chemistry, Northwestern University

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## Current Position

Postdoctoral Fellow  
**Northwestern University** (2020 - Present)  
Department of Chemistry  
Advisor: **Prof. George C. Schatz**

## Education

PhD  
MPhil & MS  
**Yale University** (Spring 2020)  
School of Engineering & Applied Science  
Department of Chemistry  
Advisor: **Prof. Victor S. Batista**  
Thesis Title: Studies on electron transfer in weakly coupled systems

MSc  
**Jadavpur University**  
Department of Instrumentation  
Advisor: Prof. Arun K. Pal  
Thesis Title: BN / Pd composite films for liquid petroleum gas sensing

BSc  
**University of Calcutta**  
Department of Physics  
Minor: Mathematics & Electronics

## Publications

Peer-reviewed Journals  
Updated list available on **Google Scholar** [🌐]

**23.** Silver Nanoparticle Synthesis in Glycerol by Low-pressure Plasma Driven Electrolysis: The Roles of Free Electrons and Photons  
Chi Xu, Subhajyoti Chaudhuri, Julian Held, Himashi Andaraarachchi, George C Schatz, Uwe Kortshagen  
**J. Phys. Chem. Lett.** 2023 (In Press)

**22.** Observing Similarities and Differences in the Properties of Isostructural Niobium(V)/Tantalum(V) Coordination Compounds with Strong Pi-donor Ligands  
Maxwell H Furigay\*, Subhajyoti Chaudhuri\*, Chenshuai Li, Jiawang Zhou, Pragati Pandey, Robert Higgins, Himanshu Gupta, Patrick Carroll, Michael R Gau, Jessica Anna, George C Schatz, Eric J Schelter  
**Inorg. Chem.** 2023 (In Press)

\* Contributed equally

**21.** A Reaction Mechanism for Plasma Electrolysis of AgNO<sub>3</sub> Forming Silver Nanoclusters and Nanoparticles

Astrid L Raisanen, Chelsea M Mueller, Subhajyoti Chaudhuri, George C Schatz, Mark J Kushner

**J. Appl. Phys.** 2022, 132, pp 203302 [🌐]

**20.** Tantalum, Easy as Pi: Understanding Differences in Metal-Imido Bonding Towards Improving Ta/Nb Separations

Alexander B Weberg\*, Subhajyoti Chaudhuri\*, Thibault Cheisson, Christian Uruburo, Ekaterina Lapsheva, Pragati Pandey, Michael Gau, Patrick Carroll, George C Schatz, Eric J Schelter

**Chem. Sci.** 2022, 13, pp 6796-6805 [🌐]

\* Contributed equally | Front Cover

**19.** 300-fold conductivity increase in microbial cytochrome nanowires due to 5 temperature-induced restructuring of hydrogen bonding networks

Peter J. Dahl, Sophia M. Yi, Yangqi Gu, Atanu Acharya, Catharine Shipps, Jens Neu, J. Patrick O'Brien, Uriel N. Morzan, Subhajyoti Chaudhuri, Matthew J. Guberman-Pfeffer, Dennis Vu, Sibel Ebru Yalcin, Victor S. Batista, Nikhil S. Malvankar

**Sci. Adv.** 2022, 8, eabm7193 [🌐]

**18.** Selective Reduction of Niobium(V) Species to Promote Molecular Niobium/Tantalum Separation

Maxwell H. Furigay, Subhajyoti Chaudhuri, Sean M. Deresh, Alexander B. Weberg, Pragati Pandey, Patrick J. Carroll, George C. Schatz, and Eric J. Schelter

**Inorg. Chem.** 2022, 61, 1, pp 23-27 [🌐]

**17.** A Conductive Metal-Organic Framework Photoanode

Brian Pattengale, Jessica Freeze, Matthew Guberman-Pfeffer, Ryotaro Okabe, Sarah Ostresh, Subhajyoti Chaudhuri, Victor S. Batista, Charles Schmuttenmaer

**Chem. Sci.** Edge Article, 2020, 11, pp 9593-9603 [🌐]

**16.** Electric Field Stimulates Production of Highly Conductive Microbial OmcZ Nanowires  
Sibel Ebru Yalcin, J. Patrick O'Brien, Yangqi Gu, Krystle Reiss, Sophia M. Yi, Ruchi Jain, Vishok Srikanth, Peter J. Dahl, Winston Huynh, Dennis Vu, Atanu Acharya, Subhajyoti Chaudhuri, Tamas Varga, Victor S. Batista, Nikhil S. Malvankar

**Nat. Chem. Biol.** 2020, 16, pp 1136-1142 [🌐]

**15.** Decelerating Charge Recombination Using Fluorinated Porphyrins in N,N-bis(3,4,5-trimethoxy phenyl)aniline - Aluminum(III) Porphyrin - Fullerene Reaction Center Models  
Niloofer Zarrabi, Sairaman Seetharaman, Subhajyoti Chaudhuri, Noah Holzer, Victor S. Batista, Art van der Est, Francis D'Souza, Prashanth K Poddutoori

**J. Am. Chem. Soc.** 2020, 142, 22, pp 10008-10024 [🌐]

**14.** Regioselective Ultrafast Photoinduced Electron Transfer from Naphthols to Halocarbon Solvents

Subhajyoti Chaudhuri, Atanu Acharya, Erik Tj Nibbering, Victor S Batista

**J. Phys. Chem. Lett.** 2019, 10 (11), pp 2657-2662 [🌐]

- 13.** Effect of Electronic Coupling on Electron Transfer Rates from Photoexcited Naphthalenediimide Radical Anion to  $\text{Re}(\text{bpy})(\text{CO})_3\text{X}$   
 Jose F Martinez, Nathan T La Porte, Subhajyoti Chaudhuri, Alessandro Sinopoli, Youn Jue Bae, Muhammad Sohail, Victor S Batista, Michael R Wasielewski  
**J. Phys. Chem. C** 2019, 123 (16), pp 10178–10190 [🌐]
- 12.** Phenothiazine Radical Cation Excited States as Super-oxidants for Energy Demanding Reactions  
 Joseph A Christensen, Brian T Phelan, Subhajyoti Chaudhuri, Atanu Acharya, Victor S Batista, Michael R Wasielewski  
**J. Am. Chem. Soc.** 2018, 140 (15), pp 5290–5299 [🌐]
- 11.** Can TDDFT Describe Excited Electronic States of Naphthol Photoacids? A Closer Look with EOM-CCSD  
 Atanu Acharya, Subhajyoti Chaudhuri, Victor S Batista  
**J. Chem. Theory Comput.** 2018, 14 (2), pp 867–876 [🌐]
- 10.** Photoexcited Radical Anion Super-reductants for Solar Fuels Catalysis  
 Nathan T La Porte, Jose F Martinez, Subhajyoti Chaudhuri, Svante Hedström, Victor S Batista, Michael R Wasielewski  
**Coord. Chem. Rev.** 2018, 361: 98-119 [🌐]
- 9.** Electron Transfer Assisted by Vibronic Coupling from Multiple Modes  
 Subhajyoti Chaudhuri\*, Svante Hedström, Dalvin D Méndez-Hernández, Heidi P Hendrickson, Kenneth A Jung, Junming Ho, Victor S Batista  
**J. Chem. Theory Comput.** 2017, 13 (12), pp 6000–6009 [🌐]  
 \* Corresponding author
- 8.** Thousandfold Enhancement of Photoreduction Lifetime in  $\text{Re}(\text{bpy})(\text{CO})_3$  via Spin-Dependent Electron Transfer from a Perylenediimide Radical Anion Donor  
 Svante Hedström\*, Subhajyoti Chaudhuri\*, Nathan T La Porte, Benjamin Rudshteyn, Jose F Martinez, Michael R Wasielewski, Victor S Batista  
**J. Am. Chem. Soc.** 2017, 139 (46), pp 16466–16469 [🌐]  
 \* Contributed equally
- 7.** Linker Length-Dependent Electron-injection Dynamics of Trimesitylporphyrins on  $\text{SnO}_2$  Films  
 Shin Hee Lee, Kevin P Regan, Svante Hedström, Adam J Matula, Subhajyoti Chaudhuri, Robert H Crabtree, Victor S Batista, Charles A Schmuttermaer, Gary W Brudvig  
**J. Phys. Chem. C** 2017, 121 (41), pp 22690–22699 [🌐]
- 6.** Ultrafast Photo-induced Charge Transfer of 1-naphthol and 2-naphthol to Halocarbon Solvents  
 Subhajyoti Chaudhuri, Benjamin Rudshteyn, Mirabelle Prémont-Schwarz, Dina Pines, Ehud Pines, Dan Huppert, Erik TJ Nibbering, Victor S Batista  
**Chem. Phys. Lett.** 2017, 683:49-56 [🌐]  
 Ahmed Zewail Commemoration Issue

**5.** Fundamental Role of Oxygen Stoichiometry in Controlling the Band Gap and Reactivity of Cupric Oxide Nanosheets

Zachary S Fishman, Benjamin Rudshteyn, Yulian He, Bolun Liu, Subhajyoti Chaudhuri, Mikhail Askerka, Gary L Haller, Victor S Batista, Lisa D Pfefferle

**J. Am. Chem. Soc.** 2016, 138 (34), pp 10978–10985 [🌐]

**4.** Facile Solvolysis of a Surprisingly Twisted Tertiary Amide

Aaron J Bloomfield, Subhajyoti Chaudhuri, Brandon Q Mercado, Victor S Batista, Robert H Crabtree

**New J. Chem.** 2016, 40, 1974-1981 [🌐]

Front Cover

**3.** Molecular Titanium–hydroxamate Complexes as Models for TiO<sub>2</sub> Surface Binding

Bradley J Brennan, Jeffrey Chen, Benjamin Rudshteyn, Subhajyoti Chaudhuri, Brandon Q Mercado, Victor S Batista, Robert H Crabtree, Gary W Brudvig

**Chem. Commun.** 2016, 52, 2972-2975 [🌐]

**2.** Synthesis of Carbon Nano-fibers on p-Si Having Improved Temperature Sensing Capability

Shamima Hussain, Dibyendu Ghosh, Barun Ghosh, Subhajyoti Chaudhuri, Radhaballabh Bhar, Arun K Pal

**Mater. Sci. Eng. B** 2013, 178, 83–88 [🌐]

**1.** Novel BN/Pd Composite Films for Stable Liquid Petroleum Gas Sensor

Dibyendu Ghosh, Barun Ghosh, Shamima Hussain, Subhajyoti Chaudhuri, Radhaballabh Bhar, Arun K Pal

**Appl. Surf. Sci.** 2012, 263, 788–794 [🌐]

**4.** Interface passivation revealed by transient spectroscopy in 24% performance solar cell

Jafar I. Khan, Yi Yang, Jonathan Palmer, Samuel Tyndall, Subhajyoti Chaudhuri, Cheng Liu, Luke Grater, Jamie D North, Bin Chen, Ryan M Young, George C Schatz, Michael Wasielewski, Mercouri G Kanatzidis, Edward H Sargent, Dayne F Swearer

**3.** Probing Time-Resolved Plasma-Driven Solution Electrochemistry in a Falling Liquid Film Plasma Reactor

Tanubhav Srivastava, Subhajyoti Chaudhuri, Christopher Rich, George C Schatz, Renee Frontiera, Peter J Bruggeman

**2.** Selective Redox-reactive Separations of Niobium and Tantalum

Maxwell H Furigay, Qiaomu Yang, Subhajyoti Chaudhuri, Michael R Gau, George C Schatz, Eric J Schelter

**1.** Effects of Structural Constraints on Excited-state Properties in Dimeric Cu(I) Diimine Complexes

Waleed Helweh, Pyosang Kim, Zachary J Mast, Brian T Phelan, Nicholas P Weingartz, Subhajyoti Chaudhuri, Randolph P Thummel, George C Schatz, Lin X Chen

Submitted/  
In-Revision

## Awards

Ta-Nb International Study Center (TIC)	<b>Anders Gustaf Ekeberg Tantalum Prize</b> (2022) The Anders Gustaf Ekeberg Tantalum Prize ('Ekeberg Prize') is awarded annually by the T.I.C. for excellence in tantalum research and innovation. The Prize is awarded to the lead author(s) of the published paper, book or patent that is judged by an independent panel of experts to have made the greatest contribution to understanding the processing, properties or applications of tantalum. 2022 Prize awarded for Chem. Sci. 2022, 13, pp 6796-6805
AIChE	<b>AIChE Foundation Grant</b> (2022) Registration and travel award from The American Institute of Chemical Engineers to selected participants for attending the AIChE Annual Meeting.
NSF - CSSM	<b>Mentorship Award</b> (2022) Awarded by NSF Center for Sustainable Separation of Metals for demonstration of exemplary mentorship.
NSF - CSSM	<b>Sustainability Ambassador Award</b> (2022) Awarded by NSF Center for Sustainable Separation of Metals for considering and promoting sustainability in research and leading sustainability outreach efforts in the community.
Council for Lindau Nobel Laureate Meetings	<b>Young Scientist   69<sup>th</sup> Lindau Nobel Laureate Meeting (Physics)</b> (2019) Among the group of students & early career scientists selected from 88 countries to attend the 69 <sup>th</sup> Lindau Nobel Laureate Meeting. Funding: Deutsche Forschungsgemeinschaft (DFG)
ACS Publications	<b>Best Poster   Cokerfest Symposium</b> (2018) Adjudged best out of 40 posters at the Cokerfest Symposium organized by Boston University. Award Sponsor: Journal of Physical Chemistry
Yale University GSAS	<b>University Fellowship</b> (2013) First year training fellowship awarded to selected incoming graduate students in the Graduate School of Arts & Sciences
DST Govt. of India	<b>INSPIRE Fellowship</b> (2013) 5-year fellowship awarded by the Department of Science & Technology (DST), Govt. of India to students standing 1 <sup>st</sup> in the order of merit in a STEM Program at selected Universities/Institutes in India.
CSIR Govt. of India	<b>Junior Research Fellowship</b> (2012) 5-year fellowship awarded by the Council of Scientific & Industrial Research (CSIR), Govt. of India, to students scoring > 99 percentile in the National Eligibility Test (NET) for pursuing PhD in Physical Sciences.
UGC Govt. of India	<b>Lectureship</b> (2012) Awarded by the University Grants Commission (UGC), Govt. of India, to students selected through National Eligibility Test (NET) scoring > 99 percentile, deeming them eligible to be recruited as College/ University Lecturers in Physical Sciences.

Jadavpur University	<b>University Gold Medal</b> (2012) Awarded by Jadavpur University to the student standing 1 <sup>st</sup> in the order of merit.
Jadavpur University	<b>MSc Thesis Award</b> (2012) Awarded by the Department of Instrumentation, Jadavpur University to the student with the best thesis in the MSc program.
NSS Govt. of India	<b>National Merit Certificate</b> (2004 - 2006) Awarded under the National Scholarships Scheme (NSS), Govt. of India to students scoring > 99.9 percentile in the Board Examinations. Awarded for securing a rank in the top 50 out of over 500,000 students.

## Teaching Experience

2022	<b>DFT for Non-theorists</b> NSF-CSSM (virtual) Designed and taught a short course introducing the basic concepts and applications of density functional theory to a broad audience including undergraduate and graduate students, researchers, and faculty members.
2014	<b>Thermodynamics &amp; Fluid Mechanics Laboratory</b> Yale University Helped design new experiments for the lab. Held weekly teaching sessions. Graded weekly reports. Provided feedback on scientific writing (this course was also taken to fulfill writing credit requirements).
2012	<b>Thin Films &amp; Solid-State Materials</b> Jadavpur University Delivered lectures on thin-films deposition methods and design principles of photovoltaic devices. Graded weekly assignments.
2012	<b>Analytical Instrumentation Laboratory</b> Jadavpur University Held weekly laboratory sessions. Graded weekly reports.
2011	<b>Vacuum Science &amp; Technology</b> Jadavpur University Held laboratory demonstration sessions. Graded weekly reports.

## Mentorship Experience

	<b>Involved in research project design and scientific training of</b>
Graduate Students	Baxter Flor Northwestern University (2023 - present) Zachary Mast Northwestern University (2021 - present) Nikhil Chellam Northwestern University (2020 - present) Peter Dahl Yale University (2018 - 2019) Raj Basak Yale University (2015 - 2016) Yueshen Wu Yale University (2015 - 2016)
Summer Students	Michaela Polley Carleton College 2022 Max Wirtz University of Wisconsin, Platteville 2021

Visiting Student      Lu Wang    China University of Petroleum-Beijing    2020 - 2022

**Mentored undergraduate and graduate students as part of**

2022 - present      Lindau Mentoring Hub  
2021 - present      Yale Cross Campus  
2020 - present      CSSM Sustainability Ambassadors Program

## Service & Outreach

Committee Service    **Theoretical Chemistry Seminar Series**

**Organizer**    (2022 - present)

Organize and host the biweekly theoretical/ computational chemistry seminars in the Department of Chemistry at Northwestern University.

**Center for Molecular Quantum Transduction**

**Thrust Coordinator**    (2023 - present)

Northwestern University  
In charge of research updates for monthly CMQT meetings

**Center for Sustainable Separation of Metals**

**Trainee Advisory Board Member**    (2020 - 2022)

Helped design and execute outreach projects for the NSF-CSSM. Organized the annual Sustainability Ambassadors Program.

**Mathematical & Computational Methods in Quantum Chemistry**

**Organizing Committee**    (2016)

Yale University  
Organized the KI-Net sponsored conference with Prof. Victor S. Batista at Yale University.

**Yale BMS Symposium**

**Student Organizing Committee**    (2014)

Yale University  
Helped organize the annual Bristol Myers Squibb Symposium in the Department of Chemistry at Yale University.

Outreach

**NSF Critical Materials Outreach**

**Organizing Committee**    (2021 - 2023)

Designed and organized lectures and hands-on activities for K12 students in the greater Chicago area to teach them principles and methods of materials separation. Helped promote awareness about critical materials through social media content design in collaboration with the Mutter Museum, Philadelphia.

**New Haven Science Fair**

**Judge**    (2015 - 2018)

**Mentor**    (2018 - 2019)

Evaluated science projects for the Science Fair Program and helped teachers in New Haven public schools design physical science experiments.

## **Splash at Yale**

### **Instructor** (2014)

Taught "Seeing the invisible", introducing concepts of microscopy and spectroscopy to students participating in the program.

Journal Reviewer	Journal of the American Chemical Society Chemical Science Journal of Physical Chemistry Journal of Chemical Theory & Computation Applied Materials & Interfaces Chemical Physics Letters Nano-Structures & Nano-Objects Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy
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## **Conferences, Symposia & Workshops**

Talks & posters	AICHE Annual Meeting, FL, 2023 MRS Fall Meeting, MA, 2023 77 <sup>th</sup> ACS Northwest Regional Meeting, MT, 2023 AIChE Annual Meeting, AZ, 2022 DOE EFRC PI Meeting, DC, 2019 69 <sup>th</sup> Lindau Nobel Laureate Meeting, Germany, 2019 256 <sup>th</sup> ACS National Meeting, MA, 2018 Electron Donor Acceptor Interactions GRC, RI, 2018 Computational Chemistry GRC, VT, 2018 Cokerfest Symposium, MA, 2018 American Conference on Theoretical Chemistry, MA, 2017 253 <sup>rd</sup> ACS National Meeting, CA, 2017 Connecticut Valley Quantum Chemistry Meeting, CT, 2017 KI-Net Mathematical & Computational Methods in Quantum Chemistry, CT, 2016 Yale-UCL Symposium on Materials, CT, 2016
Schools	What do your data say?, Northwestern University, IL, 2020 TSRC Summer School: Fundamental Science for Alternative Energy, CO, 2016

## **Skills**

Scripting/ Programming	Bash, Python, C, Fortran Mathematica, MATLAB
Softwares	QChem, Gaussian, ADF, ORCA, NWChem, VASP, NAMD

## **Languages**

Native/ Bilingual	English, Hindi, Bengali
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## References

PhD Advisor

**Prof. Victor S. Batista**

John Gamble Kirkwood Professor  
Department of Chemistry  
Yale University  
✉ victor.batista@yale.edu

Postdoc Advisor

**Prof. George C. Schatz**

Charles E. & Emma H. Morrison Professor  
Department of Chemistry  
Northwestern University  
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Collaborators

**Prof. Nikhil S. Malvankar**

Associate Professor  
Department of Molecular Biophysics and Biochemistry  
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**Prof. Gary W. Brudvig**

Benjamin Silliman Professor  
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**Prof. Eric J. Schelter**

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More on request