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Shobhit S. Chaturvedi

Curriculum Vitae

Education

Jan. 2018 – Dec. 2022 **Doctor of Philosophy in Chemistry**, *Michigan Technological University*, Houghton, MI, USA
Advisor: Prof. Christo Z. Christov. Thesis: *"Multilevel Computational Investigation into the Dynamics and Reaction Mechanisms of Non-heme Iron and 2-Oxoglutarate Dependent Enzymes."* **M.S. in Chemistry** earned en route (2022).

2013 – 2017 **Bachelor of Technology in Chemical Engineering**, *Rashtrasant Tukadoji Maharaj Nagpur University*, Nagpur, India

Professional Experience

Aug. 2025 – Present **Postdoctoral Scholar**, *ETH Zürich*, Zürich, Switzerland, Dept. of Chemistry and Applied Biosciences (D-CHAB)
Advisor: Prof. Markus Reiher. Quantum-computing applications to biological catalysis (XPRIZE Quantum Applications — Life Sciences track); electronic-structure and multiscale modeling of an artificial metalloenzyme built on a modified cytochrome P450 scaffold (collaboration with the Ward group, University of Basel, on P450-hosted MHAT chemistry); mechanism of dinitrogen reduction by nitrogenase (as part of the **NITRO-GENESE** consortium with MPI-CEC, EPFL, and Université de Genève, combining enzymology, spectroscopy, and computational modeling on engineered and semi-synthetic nitrogenases).

Jan. 2023 – May 2025 **Postdoctoral Scholar**, *University of California, Los Angeles*, Los Angeles, CA, USA, Dept. of Chemistry and Biochemistry
Advisor: Prof. Anastassia N. Alexandrova. Established the protein intramolecular electric field as a unifying descriptor of enzyme catalysis: showed that structurally distinct chorismate mutases converge on a common electrostatic solution (JACS 2025); demonstrated that directed evolution of protoglobin systematically optimizes its active-site electric field (JACS 2024); co-developed **PyCPET** for computing heterogeneous 3D protein electric fields and their dynamics (JCTC 2025); co-trained machine-learning models that predict protein function directly from the electric-field fingerprint (JACS 2024).

Jan. 2018 – Dec. 2022 **Graduate Researcher & Teaching Assistant**, *Michigan Technological University*, Houghton, MI, USA, Dept. of Chemistry
Advisor: Prof. Christo Z. Christov. Graduate Research Assistant (May 2019 – Dec. 2022); Graduate Teaching Assistant (Jan. 2018 – May 2019). QM/MM and multiscale MD dissection of catalytic mechanisms in metalloenzymes: established how the second coordination sphere, long-range interactions, and conformational dynamics control reactivity, selectivity, and dioxygen activation in non-heme Fe(II)/2-oxoglutarate-dependent histone demethylases (PHF8, KDM4A, KDM6, KDM7), DNA-demethylation enzymes (TET2), the ethylene-forming enzyme (EFE), and Zn-dependent matrix metalloproteinases (MMP-1); demonstrated that external electric fields can switch between competing product channels in EFE.

Jun. – Dec. 2017 **Project Research Assistant**, *Indian Institute of Technology Bombay*, Mumbai, India, Dept. of Chemical Engineering
Advisor: Prof. Ateeque Malani. Molecular dynamics of aspartic-acid adsorption on different crystallographic surfaces of calcium oxalate (kidney-stone) crystals, probing how the amino acid modulates surface interactions relevant to stone formation. Preceded by a summer internship in the same group (May–Jun. 2016).

Awards & Fellowships

Graduate & Postdoctoral

2026 **ETH Zürich Focus Grant** — two-month competitive fellowship supporting preparation of an ERC Starting Grant application (CHF 10,106, 50% salary); ETH Zürich Grants Office.

2024 **Poster Presentation Award**, SoCal TheoChem 2024, UC San Diego.

2022 **Doctoral Finishing Fellowship**, Michigan Technological University.

2022 **Health Research Institute Fellowship**, Michigan Technological University.

2021 **Poster Presentation Award — 1st Place**, ACS Upper Peninsula Local Section.

2020, 2021 **Career Enrichment Grant**, Graduate Student Government, Michigan Technological University.

2020 **Outstanding Graduate Student Summer Research Award**, Dept. of Chemistry, Michigan Technological University.

2019 **Travel Grant**, Graduate Student Government, Michigan Technological University.

2018 **AAAS/Science Program for Excellence in Science Award**, American Association for the Advancement of Science.

Undergraduate

2016 **Rotary Youth Leadership Award**, Rotary Club of Nagpur.

2016 **Project Exhibition Award — 3rd Place**, NCOAT-NIRMITI, Priyadarshini Institute of Engineering & Technology.

2015 **Oral Presentation Award — 1st Place**, Unnati 15, Priyadarshini College of Engineering.

Research Grants (Computational Allocations)

Summary ~**$232,500** in NSF ACCESS HPC allocations awarded while at UCLA, across 7 awards (5 as PI, 2 as Co-PI).

2024, 2025 **Maximize ACCESS CHE160054, Co-PI (renewal)**, *NSF ACCESS*
Combined value: $158,228 ($121,706 in 2025; $36,522 in 2024), via UCLA.

2024 **Discover ACCESS CHE240077, PI**, *NSF ACCESS*
Estimated value of awarded resources: $14,838 (via UCLA).

2024 **Discover ACCESS CHE240053, PI**, *NSF ACCESS*
Estimated value of awarded resources: $14,838 (via UCLA).

2023 **Discover ACCESS BIO230147, PI**, *NSF ACCESS*
Estimated value of awarded resources: $14,838 (via UCLA).

2023 **Discover ACCESS CHE230072, PI**, *NSF ACCESS*
Estimated value of awarded resources: $14,838 (via UCLA).

2023 **Discover ACCESS CHE230069, PI**, *NSF ACCESS*
Estimated value of awarded resources: $14,838 (via UCLA).

Peer-Reviewed Publications

Summary 23 peer-reviewed journal articles (9 first-author, 1 equal-contribution first) and 1 first-author book chapter; 1 preprint. Cited **761** times; **h-index 18**, i10-index 21 (Google Scholar, Apr. 2026).

Journal Articles

2025 **(24) Chaturvedi, S. S.**, Goswami, A., Qian, J., Petersen, A., Ajmera, P., Alexandrova, A. N. "Distinct Electric Fields Enable Common Catalytic Function in Structurally Diverse Enzymes." ***J. Am. Chem. Soc.*** **147**(35), 32225–32237 (2025).

2025 **(23)** Eberhart, M. E., Alexandrova, A. N., Ajmera, P., Bim, D., **Chaturvedi, S. S.**, Vargas, S., Wilson, T. R. "Methods for Theoretical Treatment of Local Fields in Proteins and Enzymes." ***Chem. Rev.*** **125**(7), 3772–3812 (2025).

2025 **(22)** Ajmera, P., Vargas, S., **Chaturvedi, S. S.**, Hennefarth, M., Alexandrova, A. N. "PyCPET — Computing Heterogeneous 3D Protein Electric Fields and Their Dynamics." ***J. Chem. Theory Comput.*** **21**(8), 4299–4308 (2025).

2024 **(21)** Vargas, S., **Chaturvedi, S. S.**, Alexandrova, A. N. "Machine-Learning Prediction of Protein Function from the Portrait of Its Intramolecular Electric Field." ***J. Am. Chem. Soc.*** **146**(41), 28375–28383 (2024).

2024 **(20)** Thomas, M. G., Simahudeen, B. JSR., **Chaturvedi, S. S.**, Gorantla, K. R., White, W., Wildey, J., Schofield, C. J., Christov, C. Z. "The Unique Role of the Second Coordination Sphere to Unlock and Control Catalysis in Nonheme Fe(II)/2-Oxoglutarate Histone Demethylase KDM2A." ***Inorg. Chem.*** **63**(23), 10737–10755 (2024).

2024 **(19) Chaturvedi, S. S.**, Vargas, S., Ajmera, P., Alexandrova, A. N. "Directed Evolution of Protoglobin Optimizes the Enzyme Electric Field." ***J. Am. Chem. Soc.*** **146**(24), 16670–16680 (2024).

2023 **(18)** Varghese, A., Waheed, S. O., **Chaturvedi, S. S.**, DiCastri, I., LaRouche, C., Kasi, B., Lehnert, N., Li, D., Christov, C. Z., Karabencheva-Christova, T. G. "Revealing the Catalytic Strategy of FTO." ***Chem Catalysis*** **3**, 100732 (2023).

2023 **(17) Chaturvedi, S. S.**, Bim, D., Christov, C. Z., Alexandrova, A. N. "From Random to Rational: Improving Enzyme Design Through Electric Fields, Second Coordination Sphere Interactions, and Conformational Dynamics." ***Chem. Sci.*** **14**, 10997–11011 (2023).

2023 **(16)** Simahudeen, B. JSR., **Chaturvedi, S. S.**, Warner, C., Wildey, J., White, W., Thompson, M., Schofield, C. J., Christov, C. Z. "Catalysis by KDM6 Histone Demethylases — A Synergy Between the Non-Heme Iron(II) Center, Second Coordination Sphere, and Long-Range Interactions." ***Chem. Eur. J.*** **29**(51), e202301305 (2023). *(Front cover.)*

2023 **(15) Chaturvedi, S. S.**, Simahudeen, B. JSR., Ramanan, R., Rankin, J. A., Hu, J., Hausinger, R. P., Christov, C. Z. "Can an External Electric Field Switch Between Ethylene Formation and L-Arginine Hydroxylation in the Ethylene-Forming Enzyme?" ***Phys. Chem. Chem. Phys.*** **25**, 13772–13783 (2023).

2023 **(14) Chaturvedi, S. S.**, Thomas, M. G., Wildey, J., Warner, C., White, W., Schofield, C. J., Hu, J., Hausinger, R. P., Karabencheva-Christova, T. G., Christov, C. Z. "Dioxygen Binding Is Controlled by the Protein Environment in Non-Heme Fe(II) and 2-Oxoglutarate Oxygenases: A Study on Histone Demethylase PHF8 and an Ethylene-Forming Enzyme." ***Chem. Eur. J.*** **29**(24), e202300138 (2023).

2022 **(13) Chaturvedi, S. S.**, Simahudeen, B. JSR., Waheed, S. O., Wildey, J., Warner, C., Schofield, C. J., Karabencheva-Christova, T. G., Christov, C. Z. "Can Second Coordination Sphere and Long-Range Interactions Modulate Hydrogen Atom Transfer in a Non-Heme Fe(II)-Dependent Histone Demethylase?" ***JACS Au*** **2**(9), 2169–2186 (2022).

2022 **(12)** Waheed, S. O., Varghese, A., **Chaturvedi, S. S.**, Karabencheva-Christova, T. G., Christov, C. Z. "How Human TET2 Enzyme Catalyzes the Oxidation of Unnatural Cytosine Modifications in Double-Stranded DNA." ***ACS Catal.*** **12**(9), 5327–5344 (2022).

2022 **(11)** Varghese, A., **Chaturvedi, S. S.**, DiCastri, B., Mehler, E., Fields, G. B., Karabencheva-Christova, T. G. "Effects of the Nature of Metal Ion, Protein and Substrate on the Catalytic Center in Matrix Metalloproteinase-1: Insights from Multilevel MD, QM/MM and QM Studies." ***ChemPhysChem*** **23**(4), e202100680 (2022). *(Front cover and cover profile.)*

2021 **(10)** Varghese, A., **Chaturvedi, S. S.**, Fields, G. B., Karabencheva-Christova, T. G. "A Synergy Between the Catalytic and Structural Zn(II) Ions and the Enzyme and Substrate Dynamics Underlies the Structure–Function Relationships of Matrix Metalloproteinase Collagenolysis." ***J. Biol. Inorg. Chem.*** **26**(5), 583–597 (2021).

2021 **(9)** Waheed, S. O., **Chaturvedi, S. S.**, Karabencheva-Christova, T. G., Christov, C. Z. "Catalytic Mechanism of Human Ten-Eleven Translocation-2 (TET2) Enzyme: Effects of Conformational Changes, Electric Field, and Mutations." ***ACS Catal.*** **11**(7), 3877–3890 (2021).

2021 **(8) Chaturvedi, S. S.**, Ramanan, R., Hu, J., Hausinger, R. P., Christov, C. Z. "Atomic and Electronic Structure Determinants Distinguish Between Ethylene Formation and L-Arginine Hydroxylation Reaction Mechanisms in the Ethylene-Forming Enzyme." ***ACS Catal.*** **11**(3), 1578–1592 (2021).

2020 **(7)** Waheed, S. O., Ramanan, R., **Chaturvedi, S. S.**, Lehnert, N., Schofield, C. J., Christov, C. Z., Karabencheva-Christova, T. G. "Role of Structural Dynamics in Selectivity and Mechanism of Non-Heme Fe(II) and 2-Oxoglutarate-Dependent Oxygenases Involved in DNA Repair." ***ACS Cent. Sci.*** **6**(5), 795–814 (2020). *(Supplementary cover.)*

2020 **(6)** Ramanan, R., **Chaturvedi, S. S.**, Lehnert, N., Schofield, C. J., Karabencheva-Christova, T. G., Christov, C. Z. "Catalysis by the JmjC Histone Demethylase KDM4A Integrates Substrate Dynamics, Correlated Motions, and Molecular Orbital Control." ***Chem. Sci.*** **11**(36), 9950–9961 (2020).

2020 **(5) Chaturvedi, S. S.**, Ramanan, R., Lehnert, N., Schofield, C. J., Karabencheva-Christova, T. G., Christov, C. Z. "Catalysis by the Non-Heme Iron(II) Histone Demethylase PHF8 Involves Iron Center Rearrangement and Conformational Modulation of Substrate Orientation." ***ACS Catal.*** **10**(2), 1195–1209 (2020).

2019 **(3) Chaturvedi, S. S.**, Ramanan, R., Waheed, S. O., Ainsley, J., Evison, M., Ames, J. M., Schofield, C. J., Karabencheva-Christova, T. G., Christov, C. Z. "Conformational Dynamics Underlies Different Functions of Human KDM7 Histone Demethylases." ***Chem. Eur. J.*** **25**(21), 5422–5426 (2019).

2019 **(2)** Waheed, S. O., Ramanan, R., **Chaturvedi, S. S.**, Ainsley, J., Evison, M., Ames, J. M., Schofield, C. J., Karabencheva-Christova, T. G., Christov, C. Z. "Conformational Flexibility Influences Structure–Function Relationships in Nucleic Acid N-Methyl Demethylases." ***Org. Biomol. Chem.*** **17**, 2223–2231 (2019).

2018 **(1)** Ainsley, J., **Chaturvedi, S. S.**, Karabencheva-Christova, T. G., Tanasova, M., Christov, C. Z. "Integrating Molecular Probes and Molecular Dynamics to Reveal Binding Modes of GLUT5 Activatory and Inhibitory Ligands." ***Chem. Commun.*** **54**, 9917–9920 (2018). *(Equal contribution with first author.)*

Book Chapters

2019 **(4) Chaturvedi, S. S.**, Ramanan, R., Waheed, S. O., Karabencheva-Christova, T. G., Christov, C. Z. "Structure–Function Relationships in KDM7 Histone Demethylases." In ***Adv. Protein Chem. Struct. Biol.*** **117**, 113–125. Academic Press (2019).

Preprints

2025 Ajmera, P., Farley, L., Minnetian, N., King, R., Jayasekara, H., **Chaturvedi, S. S.**, Yang, J., Alexandrova, A. N., Rovis, T. "Designing an Artificial Metalloenzyme for Re-based CO_2 Photoreduction." ***ChemRxiv*** (2025). DOI: 10.26434/chemrxiv-2025-mhw1f.

Oral Presentations

2024 **Chaturvedi, S. S.**, Vargas, S., Ajmera, P., Alexandrova, A. N. "Directed Evolution Optimizes Electric Field in Protoglobin for Non-Native Catalysis." Gordon Research Seminar — Bioinorganic Chemistry, Ventura, CA.

2023 **Chaturvedi, S. S.**, Vargas, S., Alexandrova, A. N. "Directed Evolution Optimizes Electric Field in Protoglobin for Non-Native Catalysis." SoCal TheoChem 2023, UCLA, CA.

2022 **Chaturvedi, S. S.**, Hu, J., Hausinger, R. P., Christov, C. Z. "Factors Influencing Ethylene Production in the Ethylene-Forming Enzyme." ACS National Meeting, Fall 2022, Bioinorganic Chemistry Session (Virtual).

Teaching

Spring 2026 **Teaching Assistant — *Quantenchemie* (Quantum Chemistry)**, *ETH Zürich*, Zürich, Switzerland, Instructor: Prof. Markus Reiher

Spring 2019 **Graduate Teaching Assistant — CH3521 Physical Chemistry Lab II**, *Michigan Technological University*

Fall 2018 **Graduate Teaching Assistant — CH3511 Physical Chemistry Lab I**, *Michigan Technological University*

Spring 2018 **Graduate Teaching Assistant — CH1151 University Chemistry Lab I**, *Michigan Technological University*

Mentoring

UCLA — Postdoctoral Scholar (2023–2025)

Graduate mentorship: trained three Alexandrova-Lab graduate students — P. Ajmera, A. Goswami, A. Petersen — in electric-field analysis, QM/MM reaction mechanisms, molecular dynamics, and ML on protein electric fields. Mentee contributions supported two Chaturvedi-led publications (*Distinct Electric Fields*, JACS 2025, #24; *Directed Evolution of Protoglobin*, JACS 2024, #19); advised on manuscript preparation, peer-review responses, and fellowship / NSF ACCESS applications.

Undergraduate mentorship: J. Qian (co-author on *Distinct Electric Fields*, #24) and H. Jayasekara (co-author on artificial-metalloenzyme preprint).

Experimental collaborations: collaborated with the Yang group (UC Irvine) and the Rovis group (Columbia) on a cross-institutional artificial-metalloenzyme project targeting Re(I)-catalyzed CO_2 photoreduction in a designed protein scaffold (ChemRxiv preprint, 2025).

Michigan Tech — Graduate Researcher (2018–2022)

Undergraduate mentorship: J. Wildey, C. Warner, W. White — contributions yielded two Chaturvedi-led publications (JACS Au 2022, #13; Chem. Eur. J. 2023, #14) and two ACS poster presentations.

Ph.D. onboarding: mentored three incoming Ph.D. students in force-field parameter development, molecular dynamics, and QM/MM workflows (HPC job setup, mechanism analysis, data interpretation).

Experimental collaborations: connected junior lab members with experimental collaborators at Michigan State (Hu / Hausinger groups) on the ethylene-forming enzyme and Oxford (Schofield group) on 2-oxoglutarate-dependent enzymes to validate computational predictions.

Service & Involvement

Peer Review

Journals — Reviewer for *JACS Au*, *J. Phys. Chem. B*, and *ACS Phys. Chem. Au*.

Departmental & Organizational

Sep. 2018 – May 2019 — **Chemistry Department Representative**, *Graduate Student Government, Michigan Technological University*

Sep. 2018 – May 2019 — **Member, Academic Committee**, *Graduate Student Government, Michigan Technological University*

Jun. 2015 – May 2016 — **Secretary**, *Rotaract Club, Priyadarshini Institute of Engineering & Technology*

Jun. 2015 – May 2016 — **Head of Abhyudaya Board**, *Dept. of Chemical Engineering, Priyadarshini Institute of Engineering & Technology*

Professional Affiliations

Jun. 2019 – Present — American Chemical Society.

Aug. 2018 – Present — American Association for the Advancement of Science.