Shobhit S. Chaturvedi

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PROFESSIONAL EXPERIENCE

Postdoctoral Scholar
Department of Chemistry and Biochemistry, University of California, Los Angeles — January 2023 – Present
Advisor: Dr. Anastassia Alexandrova

Graduate Research Assistant
Department of Chemistry, Michigan Technological University — May 2019 – December 2022

Graduate Teaching Assistant
Department of Chemistry, Michigan Technological University — January 2018 - May 2019

Project Research Assistant
Department of Chemical Engineering, Indian Institute of Technology Bombay — June 2017 - December 2017

Summer Intern
Department of Chemical Engineering, Indian Institute of Technology Bombay — May 2016 - June 2016

EDUCATION

Doctor of Philosophy in Chemistry
Michigan Technological University, GPA 3.78/4.00 — January 2018 – December 2022
Advisor: Dr. Christo Z. Christov

Master of Science in Chemistry
Michigan Technological University, GPA 3.78/4.00 — January 2018 – December 2022
Advisor: Dr. Christo Z. Christov

Bachelor of Technology in Chemical Engineering
Rashtrasant Tukadoji Maharaj Nagpur University, CGPA 8.48/10.00 — June 2014 - May 2017

RESEARCH EXPERTISE

Hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) Simulations

- Potential energy surfaces of enzyme reaction mechanisms using adiabatic mapping
- Electronic structure analysis through molecular orbitals, natural/spin natural orbitals
- External electric field QM/MM calculations
- QM/MM molecular dynamics simulations

Classical Molecular Dynamics Simulations

- Molecular dynamics simulations of proteins, nucleic acids and crystal surfaces

- Force field parameters development for metal-containing proteins and nucleic acids
- Enzyme dynamics investigation using dynamic cross correlation and principal component analysis

Free Energy Simulations

- Free energy surfaces of enzyme reactions via QM/MM metadynamics
- Free energy calculations of ligand binding to surface/protein via molecular mechanics metadynamics and potential of mean force (PMF) umbrella sampling
- Ligand binding free energy calculations via MMPBSA/MMGBSA

Programming & Computer Administration

- Job automation and analysis using Bash scripting
- Software installations and maintenance of UNIX based high performance computers

PEER-REVIEWED PUBLICATIONS

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*, 2022, 2(9), 2169–2186.

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.*, 2022, 12(9), 5327-5344.

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.*, 2021, 23(4), e202100680. **(Selected for the front cover and cover profile)**.

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.*, 2021, 26(5), 583-597.

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.*, 2021, 11(7), 3877-3890.

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.*, 2021, 11(3), 1578-1592.

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.*, 2020, 6(5), 795-814. **(Selected for the supplementary cover image).**

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.*, 2020, 11(36), 9950-9961.

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.*, 2020, 10(2), 1195-1209.

Chaturvedi, S. S., Ramanan, R., Waheed, S. O., Karabencheva-Christova, T. G., Christov, C. Z. "Structure-function relationships in KDM7 histone demethylases", *Adv. Protein Chem. Struct. Biol.*, 2019, 117, 113-125.

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.*, 2019, 25(21), 5422-5426.

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.*, 2019, 17, 2223-2231.

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.*, 2018, 54, 9917-9920. **(Equal contribution with the first author)**.

Under Review/Submission

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", 2022, manuscript under review.

Chaturvedi, S. S., Thomas, M. G.,& Wildey, J.,# Warner, C.,# White, R.,# Schofield, C. J., Hu, J., Hausinger, R. P., Karabencheva-Christova, T. G., Christov, C. Z. "Protein Environment Controls Dioxygen Binding and 2OG Coordination Preference in Do Non-Heme Fe(II) and 2OG Dependent Oxygenases – Study on Histone Demethylase PHF8 and Ethylene Forming Enzyme", 2022, manuscript under preparation for submission.

& Graduate students, # Undergraduate students

CONFERENCE PRESENTATIONS

Oral Presentations

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.

Poster Presentations

Chaturvedi, S. S., Wildey, J.,# Warner, C.,# Karabencheva-Christova, T. G., Christov, C. Z. "Second Coordination Sphere and Long-Range Interactions as Tools for Modulating HAT in a Histone Demethylase", *ACS National Meeting*, Fall 2022, Bioinorganic Chemistry Session, Virtual.

Chaturvedi, S. S., Wildey, J.,# Warner, C.,# Karabencheva-Christova, T. G., Christov, C. Z. "Iron Center Rearrangement in Catalytic Mechanism of Human Non-Heme Iron (II) Histone Demethylase PHF8", *ACS UPLS*, Fall 2021, Marquette, USA.

Chaturvedi, S. S., Ramanan, R., Hu, J., Hausinger, R. P., Christov, C. Z. "Structural Determinants for ethylene Formation and L-Arginine Hydroxylation Reaction Mechanism in the Ethylene-Forming Enzyme", *ACS National Meeting*, Fall 2021, Bioinorganic Chemistry Session, Virtual.

Chaturvedi, S. S., Ramanan, R., Karabencheva-Christova, T. G., Christov, C. Z. "Computation Insights into Catalytic Mechanism of Nε-Methyl Lysine Demethylation by PHF8", *Michigan Technological University*, Department of Chemistry Poster Session, 2019, Houghton, USA.

Chaturvedi, S. S., Ramanan, R., Karabencheva-Christova, T. G., Christov, C. Z. "Computation Insights into Catalytic Mechanism of Nε-Methyl Lysine Demethylation by PHF8", *ACS National Meeting*, Fall 2019, Sci-Mix Session, San Diego, USA.

Chaturvedi, S. S., Ramanan, R., Karabencheva-Christova, T. G., Christov, C. Z. "Computation Insights into Catalytic Mechanism of Nε-Methyl Lysine Demethylation by PHF8", *ACS National Meeting*, Fall 2019, Bioinorganic Chemistry Session, San Diego, USA.

Undergraduate students

TEACHING

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

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

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

MENTORING

Graduate Students

- Trained three new graduate students on forcefield parameter development, Molecular Dynamics simulations, QM/MM simulations, and electronic structure analysis
- Collaborated on several research projects leading to five peer-reviewed research publications

Undergraduate Students

- Mentored and trained four undergraduate students on computational modeling, forcefield parameter development and Molecular Dynamics simulations
- Published two peer-reviewed research paper and participated in two poster presentation with two undergraduate students

INVOLVEMENT

Chemistry Department Representative
Graduate Student Government, Michigan Technological University — September 2018 - May 2019

Member of Academic Committee
Graduate Student Government, Michigan Technological University — September 2018 - May 2019

Secretary
Rotaract Club, Priyadarshini Institute of Engineering and Technology — June 2015 - May 2016

Head of Abhyudaya Board
Department of Chemical Engineering, Priyadarshini Institute of Engineering and Technology — June 2015 - May 2016

AWARDS, GRANTS & FELLOWSHIPS

Doctoral Finishing Fellowship

Michigan Technological University 2022

Health Research Institute Fellowship
Michigan Technological University 2022

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

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

Outstanding Graduate Student Summer Research Award
Department of Chemistry, Michigan Technological University 2020

Travel Grant
Graduate Student Government, Michigan Technological University 2019

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

Rotary Youth Leadership Award
Rotary Club of Nagpur 2016

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

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

PROFESSIONAL AFFILIATIONS

American Chemical Society June 2019 - Present

American Association for Advancement of Science August 2018 - Present