Saswata Dasgupta

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EMPLOYMENT

Kansas State University — **Manhattan, USA**
Assistant Professor — *August 2025 –*

University of California San Diego — **San Diego, USA**
Postdoctoral researcher — *July 2020 – June 2025*

- Under the supervision of **Prof. Francesco Paesani**

EDUCATION

The Ohio State University — **Columbus, USA**
Ph.D — *August 2014 – June 2020*

- Thesis title: **"*Ab-initio* Implementation of Ground and Excited State Resonance Raman Spectroscopy: Application to Condensed Phase and Progress Towards Biomolecules"**
  (Under the supervision of **Prof. John M. Herbert**)

IIT Madras — **Chennai, India**
M.Sc. in Chemistry — *2012 – 2014*

- Thesis title: **"Scalar couplings in solution state of spin-1 AX_2 system using multiple quantum NMR spectroscopy and spin dynamics"**
  (Under the supervision of **Prof. Narayanan Chandrakumar**)
  **Nominated for best thesis award*

Visva-Bharati University — **Santiniketan, India**
B.Sc. (Major: Chemistry) — *2009 – 2012*
Minor: Physics & Mathematics

RESEARCH EXPERIENCE

Eric and Wendy Schmidt AI in Science Postdoctoral Fellow — *2023–2025*
UC San Diego, San Diego, CA
Advisor: Prof. Francesco Paesani
Major Projects:

- *Advancing chemical reactivity in condensed phases through machine-learning*

Postdoctoral researcher — *2020–*
UC San Diego, San Diego, CA
Advisor: Prof. Francesco Paesani
Major Projects:

- *Development of accurate potential-energy functions with many-body DFT formalism*
- *Development and applications of fully polarizable QM/MB methods*

Graduate Researcher — *2015–2020*
The Ohio State University, Columbus, OH
Advisor: Prof. John Herbert
Major Projects:

- *Novel optimization technique for enzymatic reactions*
- *Implementation and simulation of femtosecond stimulated Raman spectra for chromophores*
- *Ab-initio implementation of resonance-Raman spectra and application to $e(aq)^-$*
- *Standard grids for the integration of modern density functionals*

Masters thesis *2013–2014*
Indian Institute of Technology (IIT) Madras, Chennai, India
Advisor: Prof. Narayanan Chandrakumar
Major Project:
- *Scalar couplings in solution state of spin-1 AX_2 system using multiple quantum NMR spectroscopy and spin dynamics*

Summer Project *2013*
Indian Institute of Science Education and Research (IISER) Kolkata, Kolkata, India
Advisor: Prof. Amlan K. Roy
Major Project:
- *Formation of non-symmetrical Cartesian coordinate grid for DFT*

TECHNICAL SKILLS

- **OS:** Linux, Macintosh, Windows
- **Programming languages:** C++, Python, Fortran, Unix shells
- **Computational chemistry programs:** Q-Chem (developer since v. *5.0*), ORCA, CP2K, i-Pi, LAMMPS, PLUMED
- **ML computational chemistry tools:** Allegro, DeePMD-kit, MACE, RDkit
- **Molecule visualization:** IQmol, Pymol, VMD, Chimera
- **Non-chemistry softwares:** LaTeX, MatLab, Mathematica, Adobe Illustrator.

PUBLICATIONS

*Corresponding authorships are marked with **

Published articles

17. "Intermolecular Interactions Override Chemical Intuition in Tuning Stacking and Electronic Properties of Functionalized 2D COFs" Yuanhui Pan*, **Saswata Dasgupta***, Raja Ghosh* and Francesco Paesani*, ***Chem. Mater.***, 2025, 37, 6881

16. "Sub-Nanometer Confinement Suppresses Autoionization of Water" **Saswata Dasgupta***, Suman Saha and Francesco Paesani*, ***J. Am. Chem. Soc.***, 2025, 147, 25167

15. "Nuclear quantum effects and the Grotthuss mechanism dictate the pH of liquid water" **Saswata Dasgupta***, Giuseppe Cassone and Francesco Paesani*, ***J. Phys. Chem. Lett.***, 2025, 16, 2996

14. "Eliminating imaginary vibrational frequencies in quantum-chemical cluster models of enzymatic active sites" Paige Bowling, **Saswata Dasgupta** and John M. Herbert*, ***J. Chem. Inf. Model.***, 2024, 64, 3912

13. "Effect of Aliphatic Substituents on Viscosity Sensitivity for Arylcyanoamide-based Fluorescent Dyes" Rachel S. Ehrlich, **Saswata Dasgupta**, R. Erin Jessup, Kristine L. Teppang, Alexander L. Shiao *et. al.*, ***J. Phys. Chem. B***, 2024, 128, 3946

12. "Balance between physical interpretability and energetic predictability in widely used dispersion-corrected density functionals" **Saswata Dasgupta***, Etienne Palos, Yuanhui Pan , and Francesco Paesani*, ***J. Chem. Theory Comp.*** , 2024, 20, 49

11. "Data-Driven Many-Body Potentials from Density Functional Theory for Aqueous Phase Chemistry" Etienne Palos*, **Saswata Dasgupta**, Eleftherios Lambros, and Francesco Paesani*, ***Chem. Phys. Rev.*** , 2023, 4, 011301

10. "How Good is the Density-Corrected SCAN Functional for Neutral and Ionic Aqueous Systems, and What is so Right about the Hartree-Fock Density?" **Saswata Dasgupta***, Chandra Shahi, Pradeep Bhetwal, John P Perdew* and Francesco Paesani* ***J. Chem. Theory Comp.***, 2022, 18, 4745

9. "Density Functional Theory of Water with the Machine-Learned DM21 Functional" **Saswata Dasgupta***†, Etienne Palos*†, Eleftherios Lambros*†, and Francesco Paesani* ***J. Chem. Phys***, 2022, 16, 161103 (†*Contributed equally)*

8. "Assessing the Interplay Between Functional-Driven and Density-Driven Errors in DFT Models of Water" Etienne Palos*, Eleftherios Lambros*, Steven Swee, Jie Hu, **Saswata Dasgupta** and Francesco Paesani* ***J. Chem. Theory Comp.***, 2022, 18, 3410

7. "Elevating Density Functional Theory to Chemical Accuracy for Water Simulations through a Density-Corrected Many-Body Formalism" **Saswata Dasgupta**†, Eleftherios Lambros†, John P. Perdew and Francesco Paesani* ***Nat. Commun***, 2021, 12, 1, 1-12. (†*Contributed equally)*

6. "General many-body framework for data-driven potentials with arbitrary quantum mechanical accuracy: Water as a case study" **Saswata Dasgupta**[*†], Eleftherios Lambros[*†], Etienne Palos, Steven Swee, Jie Hu and Francesco Paesani[*] ***J. Chem. Theory Comp.***, 2021, 17, 5635–5650 *([†]Contributed equally)*

5. "Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package" Epifanovsky *et. al.* ***J. Chem. Phys.***, 2021, 155, 084801.

4. "*Ab Initio* Approach to Femtosecond Stimulated Raman Spectroscopy: Investigating Vibrational Modes Probed in Excited-State Relaxation of Quaterthiophenes " **Saswata Dasgupta** and John M. Herbert* ***J. Phys. Chem. A***, 2020, 124, 31, 6356–6362.

3. "Using Atomic Confining Potentials for Geometry Optimization and Vibrational Frequency Calculations in Quantum-Chemical Models of Enzyme Active Sites" **Saswata Dasgupta** and John M. Herbert* ***J. Phys. Chem. B***, 2020, 124, 7, 1137-1147.

2. "*Ab Initio* Investigation of the Resonance Raman Spectrum of the Hydrated Electron " **Saswata Dasgupta**, Bhaskar Rana and John M. Herbert* ***J. Phys. Chem. B***, 2019, 123, 8074-8085

1. "Standard grids for high-precision integration of modern density functionals: SG-2 and SG-3" **Saswata Dasgupta** and John M. Herbert* ***J. Comp. Chem.***, 2017, 38, 869-882

TEACHING EXPERIENCE

CHM 854: Theoretical Chemistry I *Fall 2025*

Kansas State University
Instructor of Record
- Designed and taught a graduate-level course covering the foundations of quantum mechanics and theoretical chemistry.
- Created interactive assignments and assessments to strengthen both conceptual understanding and computational skills.

Physical Chemistry 4300
(Quantum Chemistry & Chemical Kinetics) *Fall 2015, 16, 17*
The Ohio State University
Graduate Teaching Associate
- Conducted weekly recitation sessions.
- Conducted weekly office hours.
- Graded homework papers, quizzes, and examination papers

General Chemistry 1220 *Spring 2015, 17*
The Ohio State University
Graduate Teaching Associate
- Conducted weekly recitation sessions.
- Conducted weekly laboratory sessions
- Conducted weekly office hours.
- Graded homework papers, laboratory reports, quizzes, and examination papers

SCHOLASTIC ACHIEVEMENTS

Wiley Computers in Chemistry Outstanding Postdoc Award **2025**
ACS Spring 2025

INSPIRE faculty fellowship **2024**
DST India

Schmidt AI in Science Postdoctoral Fellow **2023**
UC San Diego

AFOSR Scholar **2022**
ACTC

Finalist in Hayes Advanced Research Forum **2017**
Ohio-State

Qualified in GATE Examination **2014**
All India Rank: 51

Qualified in CSIR-NET **2014**
All India Rank: 19

Qualified in CSIR-NET **2013**
All India Rank: 18

Qualified in IIT-JAM **2012**
All India Rank: 98

IIT Madras Merit Scholarship **2013–2014**
Fellowship

Visva-Bharati Merit Scholarship **2010–2012**
Fellowship

CONFERENCES & PRESENTATIONS

ACS National Meeting and Exposition *2025*
San Diego, CA
- ***Oral presentation (4198071):*** *"Unveiling water dissociation in nanoconfined environments"*
- ***Oral presentation (4198003):*** *"Nuclear quantum effects and the Grotthuss mechanism dictate the pH of water"*
- ***Oral presentation (4198055):*** *"Advancing density functional theory toward chemical accuracy for reactive and non-reactive condensed phase simulations"*

APS Global Physics Summit *2025*
Anaheim, CA
- ***Oral presentation:*** *"Advancing Density Functional Theory for Chemically Accurate Reactive and Non-Reactive Condensed Phase Simulations with Machine Learning"*

AIChE Annual Meeting *2024*
San Diego, CA
- ***Oral presentation- Faculty Candidates in CoMSEF (62o):*** *"Advancing Density Functional Theory for Condensed Phase Simulations through Machine Learning and Many-Body Techniques "*

VII Colloquium on Computational Simulation in Sciences *2024*
UNAM, MX
- ***Invited Talk:*** *"Elevating Density Functional Theory Towards Chemical Accuracy for Condensed Phase Simulations through Machine Learning and Many-Body Techniques "*

Many-body workshop *2024*
Telluride, CO
- ***Oral presentation:*** *"Elevating the Accuracy of DFT for Condensed Phase Simulations through Machine Learning and Many-Body Techniques "*

Futures of Chemistry Symposium *2024*
TIFR Mumbai
- ***Invited Talk:*** *"Elevating Density Functional Theory Towards Chemical Accuracy for Condensed Phase Simulations through Machine Learning and Many-Body Techniques "*

Virtual mini symposium on QM/MM *2022*
Webinar
- ***Oral presentation:*** *"Data-Driven Many-Body Potentials from Density Functional Theory and a Many-Body Approach to QM/MM Simulations "*

ACTC *2022*
Palisades Tahoe, CA
- ***Poster presentation:*** *"Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism "*

WATOC *2022*
Vancouver, BC
- ***Poster presentation:*** *"Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism "*

ACS National Meeting and Exposition *2022*
San Diego, CA
- ***Oral presentation (3651217):*** *"Elevating density functional theory to chemical accuracy for water simulations through a*

density-corrected many-body formalism"
- ***Oral presentation (3654984):*** *"How good is the density-corrected SCAN functional?"*

Dow Student poster Session *2019*
Columbus, OH
- ***Poster presentation:*** *"Ab Initio investigation of the resonance Raman spectrum of the hydrated electron"*

ACS National Meeting and Exposition *2019*
Orlando, FL
- ***Oral presentation (PHYS-0582):*** *"Ab Initio calculations of the resonance Raman spectrum of the hydrated electron"*
- ***Oral presentation (COMP-0619):*** *"Novel approach to compute vibrational spectra in cluster models of enzyme active sites"*

Virtual Winter School on Computational Chemistry *2019*
Webinar
- ***Single figure presentation:*** *"On the resonance-Raman spectrum of $e(aq)^-$ and cavity model"*

50^{th} Midwest Theoretical Chemistry Conference *2018*
University of Chicago
- ***Poster presentation:*** *"An ab-initio implementation and applications of resonance-Raman spectroscopy"*

Physical Chemistry divisional Seminar *2018*
Ohio State University
- ***Oral presentation:*** *"Standard Grids for integration of modern density functionals & ab-initio implementation resonance-Raman spectroscopy"*

49^{th} Midwest Theoretical Chemistry Conference *2017*
Michigan State University
- ***Poster presentation:*** *"Standard grids for high-precision integration of modern density functionals: SG-2 and SG-3"*

OSU Hayes Forum *2017*
Ohio State University
- ***Poster presentation:*** *"Standard grids for high-precision integration of modern density functionals"*

48^{th} Midwest Theoretical Chemistry Conference *2016*
University of Pittsburgh
- ***Poster presentation:*** *"Standard Grids For high-precision density functional calculations: SG-2 And SG-3"*

SERVICES

Journal reviewer
- **Journal of Chemical Theory and Computation**
- **Journal of Physical Chemistry Letters**
- **Journal of Physical Chemistry A**
- **Journal of Physical Chemistry B**
- **Journal of Chemical Physics**
- **ChemPhotoChem**
- **ACS Omega**
- **Materials Advances**

Organizer
- **Annual departmental postdoctoral research symposium,** *UC San Diego, 2024-2025*

Symposium moderator
- ***Session Moderator:*** *"PHYS: Frontiers in Vibrational Spectroscopy: Experiments and Theory"*, ***ACS Orlando, 2019***
- ***Session Moderator:*** *Midwest undergraduate computational chemistry consortium*, **Columbus, OH, 2019**
- ***Session Moderator:*** *"New Developments in QM/QM, QM/MM, and Fragmentation Methods"*, ***ACS San Diego, 2022***