Sajal Kumar Giri

Curriculum Vitae

IIT(ISM), Dhanbad, India
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Employment

March 2025 **Assistant Professor (Grade-I)**
Dec. 2024 Department of Chemistry and Chemical Biology, IIT(ISM), Dhanbad, India

Dec. 2024 **Post Doctoral Fellow**
Dec. 2021 Department of Chemistry, Northwestern University, Evanston, USA
Advisor Prof. George C. Schatz
Projects Plasmon-Driven Photocatalysis and Entangled Photons Spectroscopy

Oct. 2021 **Machine Learning Scientist**
Feb. 2021 Iambic Therapeutics (Entos Inc.), California, USA
Project Development and Implementation of Deep-Learning Models for Electronic Structure and Molecular Property Prediction

Jan. 2021 **Post Doctoral Fellow**
Aug. 2020 Max-Planck Institute for the Physics of Complex Systems, Dresden, Germany
Project Machine Learning Light-Matter Interactions
Advisor Prof. Jan-Michael Rost

Education

July 2020 **Ph.D. in Chemistry**, *Thesis defended on July 13, 2020*
Oct. 2015 Max-Planck Institute for the Physics of Complex Systems, Dresden, Germany
Thesis titled Statistical Learning for Ultrafast Light-Matter Interactions
Thesis advisor Prof. Jan-Michael Rost

Sept. 2015 **Project Assistant**
June 2015 Indian Institute of Technology, Kanpur, India
Project Classical Limit of Quantum Coherence
Advisor Prof. Srihari Keshavamurthy

May 2015 **M.Sc. in Chemistry**
July 2013 Indian Institute of Technology, Kanpur, India
Thesis titled Laser Induced Symmetry Breaking in Classical Limit
Thesis advisor Prof. Srihari Keshavamurthy

June 2013 **B.Sc. in Chemistry**
July 2010 Ramakrishna Mission Vidyamandira, Belur Math, India (Affiliated to the University of Calcutta)

Publications

16. "Plasmon dynamics in nanoclusters: Dephasing revealed by excited states evaluation", A. O. Bhasin, Y. S. Ceylan, A. D. Dillon, **S. K. Giri**, G. C. Schatz, and R. L. M. Gieseking
J. Chem. Theory Comput. 21, 17 (2025) DOI

15. "Modeling surface-enhanced Raman scattering of Au-pyrazine and Au-pyrazine-Au nanorod dimer systems with the DFTB method", **S. K. Giri**, and G. C. Schatz
J. Phys. Chem. C 128, 19270, (2024) DOI

14. "Switching of electrochemical selectivity due to plasmonic field-induced dissociation", F. M. Alcorn, **S. K. Giri**, M. Chattoraj, R. Nixon, G. C. Schatz, and P. K. Jain
Proc. Natl. Acad. Sci. (USA) 121, e2404433121 (2024) DOI

13. "Impact of classical and quantum light on donor-acceptor-donor molecules", H. Mandal*, **S. K. Giri***, S. Jovanovski, M. Zagorska, R. Ganczarczyk, T. Chiang, G. C. Schatz, T. Goodson
J. Phys. Chem. Lett. 15, 9493 (2024) [* Equal contribution] DOI

12. "Laser pulse induced second- and third-harmonic generation of gold nanorods with real-time time-dependent density functional tight binding (RT-TDDFTB) method", **S. K. Giri**, and G. C. Schatz
J. Chem. Phys. 161, 044703(2024) DOI

11. "Roadmap on data-centric materials science", S. Bauer, ..., **S. K. Giri**, ..., and M. Scheffler
Modelling Simul. Mater. Sci. Eng. 32, 063301 (2024) DOI

10. "Colors of entangled two-photon absorption", O. Varnavski, **S. K. Giri**, T. Chiang, C. J. Zeman IV, G. C. Schatz, and T. Goodson III
Proc. Natl. Acad. Sci. (USA) 120, e2307719120 (2023) DOI

9. "Photodissociation of H_2 on Ag and Au nanoparticles: Effect of size and plasmon versus interband transitions on threshold intensities for dissociation", **S. K. Giri**, and G. C. Schatz
J. Phys. Chem. C 127, 4115 (2023) DOI

8. "Manipulating two-photon absorption of molecules through efficient optimization of entangled light", **S. K. Giri**, and G. C. Schatz
J. Phys. Chem. Lett. 13, 10140 (2022) DOI

7. "Controlling thermodynamics of a quantum heat engine with modulated amplitude drivings", **S. K. Giri**, and H. P. Goswami
Phys. Rev. E 106, 024131 (2022) DOI

6. "Perspectives for analyzing non-linear photo ionization spectra with deep neural networks trained with synthetic Hamilton matrices", **S. K. Giri**, L. Alonso, U. Saalmann, and J. M. Rost
Faraday Discuss. 228, 502 (2021) DOI

5. "Purifying electron spectra from noisy pulses with machine learning using synthetic Hamilton matrices", **S. K. Giri**, U. Saalmann, and J. M. Rost
Phys. Rev. Lett. 124, 113201 (2020) DOI

4. "Nonequilibrium fluctuations of a driven quantum heat engine via machine learning", **S. K. Giri**, and H. P. Goswami
Phys. Rev. E 99, 022104 (2019) DOI

3. "Adiabatic passage to the continuum: Controlling ionization with chirped laser pulses", U. Saalmann, **S. K. Giri**, and J. M. Rost
Phys. Rev. Lett. 121, 153203 (2018) DOI

2. "Geometric phaselike effects in a quantum heat engine", **S. K. Giri**, and H. P. Goswami
Phys. Rev. E 96, 052129 (2017) DOI

1. "Single-photon ionization in intense, fluctuating pulses", **S. K. Giri**, U. Saalmann, and J. M. Rost
J. Mod. Opt. 64, 1004 (2017) DOI

Book Chapters

1. "Plasmon enhanced spectroscopy and photocatalysis", **S. K. Giri**, and G. C. Schatz
Springer, Singapore (2024) DOI

Conference Papers

2. "Getting CO_2 to react is not easy: Hitting it hard with atomic oxygen or with hot electrons", Muwen Yang, **S. K. Giri**, and G. C. Schatz, **VIRT & L-COMM 25**, (2023) DOI

1. "Few-photon strong-field ionization", U. Saalmann, Q. Ning, M. Baghery, **S. K. Giri**, and J. M. Rost, International Symposium on Ultrafast Phenomena and Terahertz Waves, **Optica Publishing Group**, (2018) DOI

Research Areas

- Machine Learning Light-Matter Chemistry
- Entangled Photons Spectroscopy of Molecules and Nanomaterials
- Polariton Chemistry

Selected Awards

2023 Qualified for **Max-Planck-India Research Partner Group**, Germany

2015 **Proficiency Medal**, IIT Kanpur, India

2010-2015 **INSPIRE Scholarship** by Department of Science and Technology, Govt. of India

2010 **Merit-Cum-Means (MCM)** Scholarship by Govt. of West Bengal, India

Skills and Expertise

- **Computer Programming Languages:** Python, Fortran 90, Matlab, and Mathematica
- **Machine Learning Methods:** Deep Learning, Convolutional Neural Network, Gaussian Process, Bayesian Optimization, Graph Neural Network, and LASSO
- **Quantum Chemistry Methods:** TDDFT, RT-TDDFT(B), and CASSCF
- **Quantum Chemistry Codes:** DFTB+, Turbomole, NWChem, Gaussian, and Orca
- **Plotting Environments:** Matplotlib, and Gnuplot
- **Others:** TensorFlow, PyTorch, Keras, RDKit, Vesta, Avogadro, Jmol, and LaTeX

Teaching Experiences

Feb. 2018 – Oct. 2017 Teaching assistant at Technical University of Dresden, Germany
Content: Statistical Thermodynamics

Feb. 2017 – Oct. 2016 Lab assistant at Technical University of Dresden, Germany

Selected Talks and Conferences

Dec. 2023 "Entanglement-enhanced molecular spectroscopy", *TCS Meeting, IIT Madras, India*

July 2023 "From plasmon driven molecular dissociation to energy transfer using real-time time-dependent density functional tight binding method", *Dynamics at Surfaces, GRC, Salve Regina University, USA*

May 2020 "Machine learning for chemistry", *Entos Inc., Los Angeles, USA*

Nov. 2019 "Quasi-resonant two-photon ionization: From controlling transitions with adiabatic passage to determining spectra", *International Workshop on Atomic Physics, Dresden, Germany*

Dec. 2018 "Machine learning for quantum control", *Quantum Dynamics in Tailored Intense Fields (QUTIF), Young Researcher Meeting, Berlin, Germany*

Apr. 2018 "Learning spectral landscapes for strong-field optimal control", *Big-Data-Driven Materials Science, Irsee, Germany*

Mar. 2018 "Learning spectral landscape with deep learning", *Deutsche Physikalische Gesellschaft (DPG) Meeting, Erlangen, Germany*

Aug. 2017 "Can ML be used to gain insight into quasi-resonant two-photon ionization?", *QUTIF International Conference, Bad Honnef, Germany*

Mar. 2017 "FEL pulse statistics and single-photon ionization", *Deutsche Physikalische Gesellschaft (DPG) Meeting, Mainz, Germany*

Feb. 2017 "Single-photon ionization in FEL pulses", *QUTIF Annual Meeting, Dresden, Germany*

Dec. 2016 "Single-photon ionization in strong, stochastically fluctuating pulses", *QUTIF Young Researcher Meeting, Göttingen, Germany*

May 2016 "Non-perturbative single-photon ionization", *QUTIF Annual Meeting, Jena, Germany*

Feb. 2016 "Quantum control of electron dynamics", *Extreme Atomic Systems, Riezlern, Austria*

Mar. 2015 "Quantum interferences and their classical limit in coherent control scenarios: Origin of classical control", *Max-Planck Institute of Microstructure Physics, Halle, Germany*

References

Prof. Jan Michael Rost
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