

List of Publications

Sajal Kumar Giri

Feb 21, 2025

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. Giesecking
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. Chatteraj, 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 H₂ 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. Saalman, 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. Saalman, 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. Saalman, **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. Saalman, 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 CO₂ 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. Saalman, Q. Ning, M. Bagheri, **S. K. Giri**, and J. M. Rost, International Symposium on Ultrafast Phenomena and Terahertz Waves, **Optica Publishing Group**, (2018) [DOI](#)