Mathematics and Computer Science Division
Argonne National Laboratory
Lemont, IL, 60439, USA.
sgulania@anl.gov
sahilgulania.github.io

Dr. Sahil Gulania

Personal Information

Nationality **Indian**
Languages **Hindi(native), English**
Email **sgulania@anl.gov**

Experience

2021–present **Post-Doctorate Scholar, Mathematics and Computer Science Division**, *Argonne National Laboratory (ANL)*, Lemont IL, USA
Developing quantum compilers, quantum error mitigation algorithm and quantum error correction algorithms. Bench-marking quantum devices as a member of QNEXT (https://www.q-next.org/) team at Argonne National Laboratory, USA.

Education

2016–2021 **Doctor of Philosophy, Chemistry**, *University of Southern California (USC)*, Los Angeles, USA
Thesis title - New electronic structure methods for electronically excited and open-shell species within the equation-of-motion coupled-cluster framework.
Defended - March 2021

2011–2016 **Integrated Master of Science (Chemistry)**, *National Institute of Science Education and Research (NISER)*, Bhubaneswar, India
Master's thesis title - Implementation of stationary point search and intrinsic reaction coordinate following algorithms for force modified potential energy surface
CGPA - 8.6/10

Experience

2016, Fall **Leading lab sections in General Chemistry (105a)**
2017, Spring **Teaching assistant in Advanced General Chemistry (115b)**
2016-present **Active Q-Chem (quantum chemistry package) developer.**

Scholarships and Academic Awards

- Recipient of the 2021 Kenneth Nobutoshi Wachi Award from the Department of Chemistry for outstanding Ph.D. research and service.
- Dornsife Graduate School Fellowship for 5-years of study at USC.
- Innovation in Science Pursuit for Inspired Research (INSPIRE) granted by Ministry of Human Resource Development (MHRD) for all 5-years of study, INDIA
- Scholarship for Higher Education from CBSE (ISPIRE) for being in top 1 % in Central Board of Secondary Education (Class XII), INDIA

Publications

1 **Free Fermions, Matchgates and the Yang-Baxter Equation**
S. Gulania
2024 *under preparation*

2 **Initial state preparation for variational quantum eigensolver using quantum-walks**
S. Gulania
2024 *under preparation*

3 **Upper bound on QAOA quantum circuit depth for 2-regular graphs using Yang-Baxter equation**
S. Gulania
2024 *under preparation*

4 **Quantum error mitigation and correction mediated by Yang-Baxter equation and artificial neural network**
S. Gulania, S. K. Gray, B. Peng, N. Govind , Y. Alexeev
2024 *arXiv:2401.17116*

5 **Hybrid algorithm for the time-dependent Hartree–Fock method using the Yang–Baxter equation on quantum computers**
S. Gulania, S. K. Gray, B. Peng, N. Govind , Y. Alexeev
Electron. Struct., **2024** *accepted*

6 **Theory, implementation, and disappointing results for two-photon absorption cross sections within the doubly electron-attached equation-of-motion coupled-cluster framework**
K. D. Nanda, S. Gulania , A. I Krylov,
J. Chem. Phys. , **2023** *158, 054102*

7 **QuYBE - An Algebraic Compiler for Quantum Circuit Compression**
S. Gulania, Z. He, B. Peng, N. Govind , Y. Alexeev,
1st ACM/IEEE International Workshop on Quantum Computing (submitted) , **2022**

8 **Quantum time dynamics employing the Yang-Baxter equation for circuit compression**
B. Peng, S. Gulania, Y. Alexeev, N. Govind
Phys. Rev. A , **2022**, *106, 012412*,

9 **MISTIQS: An open-source software for performing quantum dynamics simulations on quantum computers**
C. Powers, L. Bassman, T.M. Linker, K. Nomura, S. Gulania, R. K. Kalia, A. Nakano, P. Vashishta
SoftwareX, **2021**, *14*, 100696

10 **Coupled cluster Green's function: Past, present, and future**
B. Peng, N.P. Bauman, S. Gulania, K. Kowalski
Annual Reports in Computational Chemistry, **2021**, *17*, 23-53

11 **Dissociative electron attachment in C2H via electronic resonances**
S. Gulania and A.I. Krylov
Mol. Phys. , **2021**, *119*, e1979262

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

13 **Equation-of-motion coupled-cluster method with double electron-attaching operators: Theory, implementation, and benchmarks**
S. Gulania, E. F. Kjonstad, J. F. Stanton, H. Koch, and A. I. Krylov
J. Chem. Phys, **2021**, *154*, 114115

14 **Limitations of Hartree-Fock with quantum resources**
S. Gulania, and J. D. Whitfield
J. Chem. Phys, **2021**, *154*, 044112

15 **Domain-specific compilers for dynamic simulations of quantum materials on quantum computers**
L. Bassman, S. Gulania, C. Powers, R. Li, T. Linker, K. Liu, T. K. Satish Kumar, Rajiv K. Kalia, A. Nakano and P. Vashishta
Quantum Sci. Technol., **2021**, *6*, 014007

16 **The quest to uncover the nature of benzonitrile anion**
S. Gulania, T-C. Jagau, A. Sanov, and A. I. Krylov
Phys. Chem. Chem. Phys. **2020**, *22*, 5002 – 5010

17 **Two cycling centers in one molecule: Communication by through-bond interactions and entanglement of the unpaired electrons**
M. Ivanov, S. Gulania, and A. I. Krylov
J. Phys. Chem. Lett., **2020**, *12*, 1297 – 1304

18 **Young frames for quantum chemistry**
S. Gulania and J. D. Whitfield
arXiv:1904.10469, **2019**

19 **EOM-CC guide to Fock-space travel: The C_2 edition**
S. Gulania, T-C. Jagau and A. I. Krylov
Faraday Disc., **2019**, *217*, 514–532

20 **Bound and continuum-embedded states of cyanopolyyne anions**
W. Skomorowski, S. Gulania, and A. I. Krylov
Phys. Chem. Chem. Phys., **2018**, *20*, 4805-4817

21 **Channel branching ratios in CH_2CN^- photo detachment: Rotational structure and vibrational energy redistribution in auto-detachment**
J. Lyle, O. Wedig, S. Gulania, A. I. Krylov, and R.Mabbs
J. Chem. Phys., **2017**, *147*, 234309

Presentation and Talks

Efficient quantum time dynamics using the Yang-Baxter equation, APS March Meeting 2023, Las Vegas, CA. March 2023
(Talk)

Polynomial Depth Quantum Circuits for Time Evolution of Heisenberg Models Using the Yang-Baxter Equation, APS March Meeting 2022, Chicago, IL. March 2022
(Talk)

Equation of motion - double electron attachment, Sanibel Symposium, St. Simons Island, GA. February 2020
(Poster)

Benzonitrile: dipole bound state vs valence anion, Utah Workshop, Park City, UT. September 2019
(Poster)

Dissociative Electron Attachment leading to Fock space traverse ($C_2H \rightarrow C_2 + H$), Pacific Conference on Spectroscopy and Dynamics, San Diego. January 2019
(Poster)

Dissociative electron attachment leading to excited C_2 anion in micro wave-activated CH_4/H_2 plasma, Gordon Research Conference, Stonehill College in Easton MA. July 2018
(Poster)

Electronic structure of cyanopolyyne anions: A computational study of valence and dipole bound states, Pacific Conference on Spectroscopy and Dynamics, San Diego. January 2018
(Poster)

Electronic Structure of negative Ions (CN^- and C_3N^-), SoCal TheoChem 2.0, University of California, Irvine. May 2017
(Poster)

References

Dr. Yuri Alexeev
Computational Scientist
Argonne National Laboratory
Lemont, Illinios, USA
email: yuri@anl.gov

Dr. Stephen K. Gray
Scientist
Center for Nanoscale Materials, Argonne National Laboratory,
Lemont, Illinios, USA
email: gray@anl.gov

Dr. Niranjan Govind
Scientist (Chemical Physics Theory)
Pacific Northwest National Laboratory
Richland, Washington, USA
email: niri.govind@pnnl.gov

Dr. Anna Krylov
Gabilan Distinguished Professor in Science and Engineering and Professor of Chemistry
University of Southern California
Los Angeles, California, USA
email: krylov@usc.edu

Dr. James Daniel Whitfield
Assistant Professor
Department of Physics and Astronomy
Dartmouth College
Hanover, New Hampshire, USA
email: james.d.whitfield@dartmouth.edu