Junjie Li, PhD

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Research Associate
Texas Advanced Computing Center

github.com/nicejunjie
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PhD in chemical physics, expert in electronic structure theory, ab initio molecular dynamics, quantum nuclear dynamics, scientific computing and High-Performance Computing (HPC). Researcher at Texas Advanced Computing Center focusing on accelerating broader range of scientific research with HPC. 10+ years' experience with HPC and scientific computing, contributor to Gaussian quantum chemistry software, 5+ years of service as secretary of SPEC High Performance Group.

Experience

Research Associate **Dec 2020 — Present**
Texas Advanced Computing Center, The University of Texas at Austin ***Austin, TX, United States***

- Performance evaluation of emerging HPC platforms.
- Characterize and improve performance of key chemistry and physics codes for Leadership Class Computing Facility funded by National Science Foundation.
- Provide technical consultations to domain scientists to improve scientific computing software.

Secretary of SPEC High Performance Group (HPG) **Jan 2017 — Present**
Standard Performance Evaluation Cooperation (SPEC) ***Global HPC Consortium***

- Lead a group of industry leading companies and prestigious research institutions across the world for SPEChpc™ 2021 benchmark development.
- Organize SPEC tutorials and workshops at academic conferences.
- Review benchmark reports submitted to HPG for publication.
- Advocate application benchmarks based HPC ranking.

Visiting Scholar **Sep 2018 — Oct 2018**
Technische Universität Dresden (TUD) ***Dresden, Germany***

- Analyze performance characteristics of SPEC benchmarks with Score-P and Vampir.
- Port key scientific codes at TUD into SPEC benchmark.

Principal System Analyst **Jul 2016 — Dec 2020**
Indiana University ***Indianapolis, IN, United States***

- Worked with 20+ research groups from neuroimaging, genomics, statistics, chemistry, physics, weather, finance, medical informatics to facilitate efficient use of advanced computing facilities:
  - Optimize pipeline and workflow for performance and throughput.
  - Accelerate computing using OpenACC on GPU.
  - Parallelize serial codes, tremendous speed up on IU's large HPC.
- Performance benchmark for popular and emerging HPC platforms.

Data Analyst **Feb 2016 — Jun 2016**
Megaputer Intelligence ***Bloomington, IN, United States***

- Utilized machine learning based big data analytics to detect emerging issues on medical devices from vast unstructured text reports in FDA database.

Education

Ph.D. in Chemical Physics
Indiana University Bloomington*, Indiana, United States.* Sep 2009 —Dec 2015

- Develop new quantum chemistry methods and algorithms for Gaussian:
  - Established innovative post-HF electronic structure method for potential surface construction during quantum nuclear dynamics. The non-orthogonal configuration interaction is calculated based on selected principal electronic states and 2e-integral is greatly simplified by introducing grid basis functions. Reduced exponential scaling to $O(N^3)$-$O(N^4)$.
  - Designed and implemented fragment-based linear scaling electronic structure method for ab initio dynamics, greatly reduced computational cost for large scale dynamics on molecular clusters and biomolecules.
  - In charge of the maintenance of 200k+ lines of code in the ab initio molecular dynamics module in Gaussian.
- Employed ab initio molecular dynamics methods in the study of proton transfer reactions and high accuracy simulations of molecular vibrational spectroscopy for highly non-harmonic systems

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B.Eng. in Applied Chemistry
***East China University of Science and Technology**, Shanghai, China* Sep 2005 — Jun 2009

- Excellent Graduates in Science and Technology.
- Thesis: DFT+U study of photochemical activity of TiO_2 Surface.

Professional Activities

- Committee member of SuperComputing Conference Reproducibility Special Journal 2022 — present
- Committee member of SuperComputing (SC) Conference Student Cluster Competition 2021 — present
- Reviewer for Journal of Molecular Modeling (JMM) 2021 — present
- Reviewer for Future Generation Computer Systems (FGCS) 2021 — present
- Reviewer for Transactions on Parallel and Distributed Systems (TPDS) 2021 — present
- Committee member of Extreme Science and Engineering Discovery Environment (XSEDE) 2021 — present
- Committee member of International Workshop on Extreme Heterogeneity Solutions (ExHET) 2021 — present
- Committee member of SuperComputing Conference ACM Undergraduate Posters 2020
- Committee member of Practice Experience in Advanced Research Computing (PEARC) 2019 — present
- Reviewer for Exploring Clouds for Acceleration of Science (E-CAS) 2019
- Committee member of Practice Experience in Advanced Research Computing (PEARC) 2019 — present
- Reviewer for International Journal of Computational Science and Engineering (IJCSE) 2018
- Reviewer for *OpenACC for Programmers* Book 2017

Award

SPECtacular Award for SPEChpc 2021 benchmark development by Standard Performance Evaluation Corporation (SPEC).
- SPEC is a premier organization formed to develop and maintain computer benchmarks, the organization contains more than 140 members from industrial and academia. The SPECtacular award is the highest honor given by the organization to recognize key contributions to the community.

Conference Tutorials

- H. Brunst, N. Hagerty, R. Henschel, **J. Li**, V. Vergara, S. Wienke. Using the New SPEChpc 2021 Scientific Application Benchmark Suites for the Evaluation of HPC Ecosystems. Tutorial at ISC High Performance 2022 Conference, Berlin, Germany May-2022.
- S. Chandrasekaran, R. Henschel, **J. Li**, V. Vergara, J. Cheng. Using the new SPEC HPC2021 Scientific Application Benchmark Suite. Tutorial at SC20 Conference, Virtual, Nov-2020.
- R. Henschel, **J. Li**, V. Vergara, M. Gimenes, S. Wienke. Using the SPEC HPG Benchmarks for Better Analysis and Evaluation of Current and Future HPC Systems. Tutorial at SC19 Conference, Denver, CO. Nov-2019.
- **J. Li** and V. Vergara. Using the SPEC HPG Benchmarks for Better Analysis and Evaluation of Current and Future HPC Systems. Tutorial at Practice Experience in Advanced Research Computing, Chicago, IL. Jul-2019.
- **J. Li** and Swen Bohm. Using the SPEC HPG Benchmarks for Better Analysis and Evaluation of Current and Future HPC Systems, Tutorial at ACM International Conference on Supercomputing, Phoenix, AZ. Jun-2019.

Publications

- **J. Li** and SPEC High Performance Group. SPEChpc 2021 Benchmark Suites for Modern HPC Systems. Accepted to 13th ACM/SPEC International Conference on Performance Engineering (ICPE 2022), Beijing, China
- H. Brunst, S. Chandrasekaran, F. Ciorba, N. Hagerty, R. Henschel, G. Juckeland, **J. Li**, V. Vergara, S. Wienke, M. Zavala. First Experiences in Performance Benchmarking with the New SPEChpc 2021 Suites. Accepted to 22nd IEEE/ACM International Symposium on Cluster, Cloud and Internet Computing (CCGrid 2022), Taormina, Italy.

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- Q. Wen, S. L. Risacher, L. Xie, **J. Li**, J. Harezlak, M. R. Farlow, F. W. Unverzagt, S. Gao, L. G. Apostolova, A. J. Saykin, Y. Wu. Tau-Related White-Matter Allterations Along Spatially Selective Pathways. Neuroimage. 2021 226, 117560
- S. Michael, S. Teige, **J. Li**, J. M. Lowe, G. Turner, R. Henschel. Performance Characteristics of Virtualized GPUs for Deep Learning. 2020 IEEE/ACM International Workshop on Interoperability of Supercomputing and Cloud Technologies (SuperCommpCloud), Atlanta, GA, USA, 2020, pp. 14-20.
- J. Zhao, Y. Si, Z. Han, **J. Li**, W. Guo, Y. Fu. An Organic-Inorganic Hybrid Cathode Based on S-Se Dynamic Covalent Bonds. Angewandte Chemie International Edition. 2020 59(7), 2654
- Q. Wen, S. M. Mustafi, J. Harezlak, **J. Li**, S. L. Risacher, J. D. West, E. F. Tallman, M. R. Farlow, F. W. Unverzagt, L. G. Apostolova, A. J. Saykin, Y. Wu. White-Matter Alterations in Early-Stage Alzheimer's Disease: A Tract-Specific Study. Alzheimer's & Dementia. 2019 11, 576.
- D. Wang, Y. Si, **J. Li** and Y. Fu. Tuning the Electrochemical Behavior of Organodisulfides in Rechargeable Lithium Batteries Using N-containing Heterocycles. Journal of Materials Chemistry A. 2019 7(13), 7423
- W. Kong, X. Zhang, B. Chang, Y. Zhou, S. Zhang, G. He, B. Yang and **J. Li**. Fabrication of B doped g-C3N4/TiO2 Heterojunction for Efficient Photoelectrochemical Water Oxidation. Electrochimica Acta. 2018 282 767.
- C. Haycraft, **J. Li** and S. S. Iyengar. Efficient, 'On-the-fly', Born-Oppenheimer and Car-Parrinello-type Dynamics with Coupled Cluster (CCSD) Accuracy Through Fragment Based Electronic Structure. Journal of Chemical Theory and Computation. 2017 13(5) 1887.
- **J. Li**, A. B. Pacheco, K. Raghavachari and S. S. Iyengar. A Grotthuss-like Proton Shuttle in the Anomalous C2H3+ Carbocation: Energetic and Vibrational Properties for Isotopologues. Physical Chemistry Chemical Physics. 2016 18(42) 29395.
- **J. Li**, C. Haycraft and S. S. Iyengar. Hybrid Extended Lagrangian and Born-Oppenheimer Molecular Dynamics Within an ONIOM Based Fragmentation Energy Extrapolation Scheme. Journal of Chemical Theory and Computation. 2016 12(6) 2493.
- **J. Li** and S. S. Iyengar. Ab Initio Molecular Dynamics Using Recursive, Spatially Separated, Overlapping Model Subsystems Mixed Within an ONIOM Based Fragmentation Energy Extrapolation Technique. Journal of Chemical Theory and Computation. 2015 11(9) 3978.
- P. Phatak, J. Venderley, J. Debrota, **J. Li** and S. S. Iyengar. Active Site Dynamical Effects that Affect the Hydrogen Transfer Rate-limiting Step in the Catalysis of Linoleic Acid by Soybean Lipoxygenase-1 (SLO-1): Primary and Secondary Isotope Effects. Journal of Physical Chemistry – B. 2015 119(30) 9532.
- **J. Li**, X. Li, and S. S. Iyengar. Vibrational Properties of Hydrogen-bonded Systems Using the Multi-reference Generalization to the "on-the-fly" Electronic Structure Within Quantum Wavepacket Ab Initio Molecular Dynamics. Journal of Chemical Theory and Computation. 2014 10(6) 2265.