

Curriculum Vitae

Shao Shi (石邵)

1 Research Interests

I am interested in postdoctoral positions or PhD programs in data science, particularly those centered on the development and application of data mining algorithms. I am also open to opportunities in the chemical, biological, or physical analysis and mining of big data, with an emphasis on the use of data mining algorithms irrespective of the specific data type. My prior work in atmospheric chemistry has provided experience in developing and implementing unsupervised machine learning algorithms, clustering methods, and ensemble learning models for large-scale datasets, which I seek to apply and further develop in interdisciplinary settings to support data-driven research.

2 Contact Information

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3 Education

- **Ph.D. in Chemistry**

Southern University of Science and Technology, Shenzhen, China

Supervisor: Prof. Dr. Xin Yang (yangx@sustech.edu.cn)

Enrolled: September 2022; Expected Graduation: June 2026

GPA: 3.78/4.00

- **B.Sc. in Environmental Science**

Southern University of Science and Technology, Shenzhen, China

Supervisor: Prof. Dr. Xin Yang (yangx@sustech.edu.cn)

Enrolled: September 2018; Graduated: June 2022

GPA: 3.71/4.00

4 Research Experience

Research focuses on atmospheric chemistry, with emphasis on single-particle measurement techniques, data mining in atmospheric big data, and ambient aerosol monitoring. Key contributions include developing innovative algorithms, conducting field measurements, and applying machine learning to enhance understanding of atmospheric processes.

4.1 I. Development of Atmospheric Single-Particle Measurement Techniques

- Developed standard-free mass calibration algorithms to accurately determine the chemical composition of atmospheric single particles, improving analytical precision and insights into atmospheric dynamics.
 1. Detailed chemical characterization of aerosols using single-particle mass spectrometry
Associated Publication:
Shi, S.*, Zhai, J., Yang, X., Ruan, Y., Huang, Y., Chen, X., Zhang, A., Ye, J., Zheng, G., Cai, B., Zeng, Y., Wang, Y., Xing, C., Zhang, Y., Fu, T.-M., Zhu, L., Shen, H., Wang, C. (2024). Technical note: Determining chemical composition of atmospheric single particles by a standard-free mass calibration algorithm. *Atmospheric Chemistry and Physics*, 24(12), 7001–7024. <https://doi.org/10.5194/acp-24-7001-2024>
 2. Quantification in single-particle mass spectrometry
Associated Manuscript (In Preparation):
Shi, S.*, et al. Entropy-Controlled Continuous Wavelet Transform for Precise Identification and Extraction of Mass Spectrum Peaks.

4.2 II. Data Mining Algorithm Development in Atmospheric Big Data

- Designed unsupervised machine learning algorithms for analyzing large-scale atmospheric datasets, enabling efficient clustering and pattern recognition.
 1. Design and application of similarity and clustering algorithms
Associated Patent:
Chinese Invention Patent: A Method, System, Terminal, and Storage Medium for Incremental Clustering of Atmospheric Aerosol Particle Mass Spectrum Datasets (一种大气气溶胶颗粒物质谱数据集的增量聚类方法、系统、终端及存储介质, Granted). Inventors: **Shi, S.***, Yang, X., et al. (Affiliated with Southern University of Science and Technology).
Associated Manuscript (In Preparation):
Shi, S.*, et al. FASC: A Flexible Adaptive Stable Clustering Algorithm for Mass Spectrometric Big Data.
 2. Implementation of data mining frameworks for tracer assessment in aerosol single particles.

4.3 III. Ambient Monitoring of Atmospheric Aerosols

- Performed comprehensive monitoring and analysis of atmospheric aerosols, including projects on respiratory deposition of ultrafine particles, ship emission impacts on air quality, and ensemble learning-based correlations between hygroscopicity and single-particle composition.

1. Quantification of pollutants, including ship-emitted particles and micro-/nano-plastics

Associated Publication:

Zhai, J., Yu, G., Zhang, J., **Shi, S.**, Yuan, Y., Jiang, S., Xing, C., Cai, B., Zeng, Y., Wang, Y., Zhang, A., Zhang, Y., Fu, T.-M., Zhu, L., Shen, H., Ye, J., Wang, C., Tao, S., Li, M., Zhang, Y., Yang, X. (2023). Impact of Ship Emissions on Air Quality in the Greater Bay Area in China under the Latest Global Marine Fuel Regulation. *Environmental Science & Technology*, 57(33), 12341–12350. <https://doi.org/10.1021/acs.est.3c03950>

Summary: Utilized online measurements and modeling to identify vanadium as a tracer for ship-emitted particles under the 0.5% sulfur fuel regulation, revealing contributions of up to 21.4% to PM and 39.5% to NO_x in summer, modulated by sea-land breezes.

2. Analysis of trace-element-containing particles and catalytic reactions at bulk and interface levels; investigation of oxalate, nitrate, and sulfate formation in single particles; assessment of health effects from ultrafine particles; and linkages between hygroscopicity and single-particle composition of atmospheric aerosols.

Associated Publications and Manuscripts:

Zhai, J., **Shi, S.**, Yang, X., Zeng, Y., Fu, T.-M., Zhu, L., Shen, H., Ye, J., Wang, C., Tao, S. (2024). Chemically Resolved Respiratory Deposition of Ultrafine Particles Characterized by Number Concentration in the Urban Atmosphere. *Environmental Science & Technology*, 58(37), 16507–16516. <https://doi.org/10.1021/acs.est.4c03279>

Summary: Employed high-resolution single-particle mass spectrometry in urban Shenzhen to quantify respiratory deposition of elemental carbon-rich ultrafine particles at approximately 2.08 billion particles per day, highlighting number-based health risks.

Shi, S.*, et al. (In Preparation). Ensemble Learning Resolved Chemical Linkage Between Hygroscopicity and Single-Particle Composition of Atmospheric Aerosols.

Summary: Applied ensemble learning models to correlate hygroscopic properties with aerosol compositions, offering insights into atmospheric dynamics, cloud formation, and climate impacts.

5 Technical Skills

- **Programming and Data Analysis:** Familiar with Python, Java, MATLAB, and R; acquainted with machine learning frameworks including PyTorch, TensorFlow, and Apache Spark; knowledgeable in unsupervised algorithms, ensemble learning, and data mining techniques.
- **Scientific Instrumentation and Methods:** Knowledgeable in physical and computational chemistry, single-particle mass spectrometry, and atmospheric aerosol monitoring techniques.

6 Awards and Honors

- National Encouragement Scholarship, Southern University of Science and Technology: 2019, 2020, 2021.

7 Publications and Patents

Publications are listed in reverse chronological order. The applicant’s name is bolded (**Shi, S.**). An asterisk (*) denotes first authorship.

7.1 Peer-Reviewed Journal Articles

1. **Shi, S.***, Zhai, J., Yang, X., Ruan, Y., Huang, Y., Chen, X., Zhang, A., Ye, J., Zheng, G., Cai, B., Zeng, Y., Wang, Y., Xing, C., Zhang, Y., Fu, T.-M., Zhu, L., Shen, H., Wang, C. (2024). Technical note: Determining chemical composition of atmospheric single particles by a standard-free mass calibration algorithm. *Atmospheric Chemistry and Physics*, 24(12), 7001–7024. <https://doi.org/10.5194/acp-24-7001-2024>
2. Zhai, J., **Shi, S.**, Yang, X., Zeng, Y., Fu, T.-M., Zhu, L., Shen, H., Ye, J., Wang, C., Tao, S. (2024). Chemically Resolved Respiratory Deposition of Ultrafine Particles Characterized by Number Concentration in the Urban Atmosphere. *Environmental Science & Technology*, 58(37), 16507–16516. <https://doi.org/10.1021/acs.est.4c03279>
3. Xing, C., Zeng, Y., Yang, X., Zhang, A., Zhai, J., Cai, B., **Shi, S.**, Zhang, Y., Zhang, Y., Fu, T.-M. (2024). Molecular characterization of major oxidative potential active species in ambient PM_{2.5}: Emissions from biomass burning and ship exhaust. *Environmental Pollution*, 355, 125291. <https://doi.org/10.1016/j.envpol.2024.125291>
4. Zeng, Y., Yang, X., Zhang, A., Yuan, X., Zhai, J., Xing, C., Cai, B., **Shi, S.**, Zhang, Y. (2024). Source-specific health effects of internally exposed organics in urban PM_{2.5} based on human serum albumin adductome analysis. *Science of The Total Environment*, 947, 176958. <https://doi.org/10.1016/j.scitotenv.2024.176958>
5. Zeng, Y., Zhang, A., Yang, X., **Shi, S.**, et al. (2024). Internal exposure potential of water-soluble organic molecules in urban PM_{2.5} evaluated by non-covalent adductome of human serum albumin. *Environment International*, 184, 108492. <https://doi.org/10.1016/j.envint.2024.108492>
6. Zhang, A., Zeng, Y., Yang, X., et al. (2023). Organic Matrix Effect on the Molecular Light Absorption of Brown Carbon. *Geophysical Research Letters*, 50(24), e2023GL106541. <https://doi.org/10.1029/2023GL106541>
7. Zhai, J., Yu, G., Zhang, J., **Shi, S.**, Yuan, Y., Jiang, S., Xing, C., Cai, B., Zeng, Y., Wang, Y., Zhang, A., Zhang, Y., Fu, T.-M., Zhu, L., Shen, H., Ye, J., Wang, C., Tao, S., Li, M., Zhang, Y., Yang, X. (2023). Impact of Ship Emissions on Air Quality in the Greater Bay Area in China under the Latest Global Marine Fuel Regulation. *Environmental Science & Technology*, 57(33), 12341–12350. <https://doi.org/10.1021/acs.est.3c03950>

8. Wang, Y., Xing, C., Cai, B., Qiu, W., Zhai, J., Zeng, Y., Zhang, A., **Shi, S.**, Zhang, Y. (2023). Impact of antioxidants on PM2.5 oxidative potential, radical level, and cytotoxicity. *Science of the Total Environment*, 905, 169555. <https://doi.org/10.1016/j.scitotenv.2023.169555>

7.2 Manuscripts in Preparation

1. **Shi, S.***, et al. FASC: A Flexible Adaptive Stable Clustering Algorithm for Mass Spectrometric Big Data.
2. **Shi, S.***, et al. Ensemble Learning Resolved Chemical Linkage Between Hygroscopicity and Single-Particle Composition of Atmospheric Aerosols.
3. **Shi, S.***, et al. Entropy-Controlled Continuous Wavelet Transform for Precise Identification and Extraction of Mass Spectrum Peaks.

7.3 Patents

1. Chinese Invention Patent: A Method, System, Terminal, and Storage Medium for Incremental Clustering of Atmospheric Aerosol Particle Mass Spectrum Datasets (一种大气气溶胶颗粒物质谱数据集的增量聚类方法、系统、终端及存储介质, Granted). Inventors: **Shi, S.***, Yang, X., et al. (Affiliated with Southern University of Science and Technology).