Shang-Chien Chen

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Profile

Algorithm prototyping engineer working on AI molecular research, computational chemistry, and molecular informatics platforms since April 2024. I have end-to-end engineering experience across algorithm prototypes, backend services, database design, frontend interaction, online deployment, and private delivery.

I mainly work on Uni-QSAR, ADMET, Uni-PK, ToxScan, NMR-Solver, and a molecular structure search database, serving as a core developer and platform owner. I am familiar with Python, RDKit, PostgreSQL, Web API design, task orchestration, authentication, MCP tool services, frontend development, and enterprise delivery workflows, and can independently turn research algorithms into commercializable platforms.

Skills

Programming and Backend Development

Experienced in Python backend development, API design, task orchestration, data processing, model service wrapping, and system integration.

Computational Chemistry and Molecular Informatics

Familiar with molecular and crystal structure data types, data flow, and processing, including structure search, feature matching, and format conversion. Experienced in building quantum chemistry workflows such as ab initio and DFT, with platform engineering experience for computational chemistry tools.

Database and Search Systems

Experienced in PostgreSQL schema design and performance tuning, including high-performance molecular structure search services built with PostgreSQL and RDKit.

Frontend and Platform Engineering

Able to build research platform interfaces, interaction flows, and integrated user-facing workflows.

Productization and Commercial Delivery

Participated in commercial platform capabilities including authentication, IAM tenant architecture, private deployment, and customer delivery support.

Project Management and Collaboration

Experienced in technical leadership and project execution, coordinating frontend, backend, algorithm, deployment, and customer requirements to move platforms from prototypes to production use.

Work Experience

Algorithm Prototyping Engineer

DP Technology | 2024.04 - Present

Responsible for the development, construction, deployment, and commercialization support of AI drug discovery and computational chemistry platforms, participating in the full process from prototype validation to platform delivery.

Main responsibilities:

- Developed and iterated Uni-QSAR, ADMET, Uni-PK, ToxScan, NMR-Solver, and related platforms, turning algorithm tools into interactive, callable, and deployable products.
- Built frontend interaction flows to improve molecule upload, task submission, result review, and data analysis experiences for research users.
- Developed backend databases and APIs covering task management, data storage, result queries, and user permission management.
- Participated in MCP tool service development, exposing platform capabilities to agents and external systems.
- Led or deeply contributed to a molecular structure search database supporting similarity search, substructure search, and complex chemical feature matching.
- Worked with customer-specific research requirements, technical validation, scenario implementation, private deployment, and delivery support.

Results:

- Helped move multiple AI drug discovery platforms from algorithm prototypes to productized and commercial use.
- Built a high-performance molecular structure search service and delivered it in customer projects.
- Supported private deployment, trial applications, and commercial validation for enterprise and research customers.
- Served as a core developer and technical driver across frontend, backend, database, task orchestration, permission management, and deployment delivery.

Projects

Participated in or led multiple AI drug discovery and computational chemistry platform projects, with a focus on turning research algorithms into interactive, callable, and deployable product capabilities.

- Uni-QSAR automated quantitative structure-activity relationship modeling platform: supports automated modeling, molecular activity prediction, model result review, and screening workflows.
- ADMET molecular property prediction platform: evaluates absorption, distribution, metabolism, excretion, and toxicity-related molecular properties for early drug screening and optimization.
- Uni-PK pharmacokinetic simulation platform: simulates concentration-time curves and helps users analyze dynamic in vivo drug behavior.
- ToxScan toxicity prediction platform: identifies potential toxicity risks during early drug discovery.
- NMR-Solver platform: supports molecular structure elucidation and NMR data analysis for structure confirmation and research workflows.
- Molecular structure search database: a PostgreSQL + RDKit service supporting similarity search, substructure search, and complex chemical feature matching.

Commercialization and Delivery

Participated in commercial platform capability development and customer project support, with experience from product feature development to customer deployment and delivery.

Capabilities include:

- Bohr photon billing support
- VIP License authorization
- Trial-domain application flows
- Authentication and permission management
- Private deployment and customer environment adaptation
- Customer issue diagnosis and technical support
- Platform validation and delivery documentation

Customers supported include:

- Huadong Medicine
- Renhe Yikang
- LONGi Green Energy
- Wanhua Chemical
- Capital Medical University

Education

Soochow University

M.S. in Materials Science and Engineering | 2018.09 - 2021.06

Coursework: materials crystallography / computational materials science / density functional theory / multiscale simulation / machine learning

Yancheng Institute of Technology

B.S. in New Energy Materials and Devices | 2014.09 - 2018.06

Coursework: fundamentals of materials science / solid-state physics / semiconductor physics / physical chemistry / new energy materials

Strengths

- Interdisciplinary technical background across AI drug discovery, cheminformatics, backend development, frontend interaction, and database engineering.
- Strong platformization ability, turning research algorithms and prototype tools into interactive, deployable, and commercializable product platforms.
- Rich engineering delivery experience across online platforms, private deployment, customer delivery, and commercial feature support.
- Deep business understanding of QSAR, ADMET, PK, toxicity prediction, NMR analysis, and molecular structure search scenarios.
- Broad ownership scope across coding, technical execution, project coordination, customer support, and platform ownership.

Publications

Date	Citation
2026-03	Cui, Y.; Ji, X.; Guo, W.; **Chen, S.**; Shen, T.; Chen, L.; Ke, G.; Jin, C.; Gao, Z.; Sun, W. **Toward Generalizable Data-Driven Pharmacokinetics with Interpretable Neural ODEs.** *Journal of Chemical Information and Modeling*, 2026, 66(5), 2640-2650. DOI: **10.1021/acs.jcim.5c02924**.
2025-10	Zhao, G.; Ou, Q.; Zhao, Z.; **Chen, S.**; Lin, H.; Ji, X.; Wang, Z.; Wang, H.; Cai, H.; Wu, L.; Lu, S.; Yang, F.; Wen, Y.; Zhang, Y.; Ma, H.; Gao, Z.; Cheng, Z.; E, W. **Virtual characterization via knowledge-enhanced representation learning: from organic conjugated molecules to devices.** *npj Computational Materials*, 2025, 11, Article 308. DOI: **10.1038/s41524-025-01788-y**.
2025-10	Fang, X.; Wang, J.; Cai, X.; **Chen, S.**; Yang, S.; Tao, H.; Wang, N.; Yao, L.; Zhang, L.; Ke, G. **MolParser: End-to-end Visual Recognition of Molecule Structures in the Wild.** In *Proceedings of the IEEE/CVF International Conference on Computer Vision (ICCV)*, 2025, pp. 24528-24538. arXiv: **2411.11098**.
2025-07	Zhao, G.; Hu, T.; Zhang, Y.; Wang, H.; Wu, L.; Lu, S.; Yang, F.; **Chen, S.**; Gao, Z.; Wang, X.; Cheng, Z. **Data-Driven Parametrization of All-Atom Force Fields for Organic Semiconductors.** *Journal of Chemical Information and Modeling*, 2025, 65(14), 7632-7638. DOI: **10.1021/acs.jcim.5c00291**.
2025-07	Ou, Q.; Wang, H.; Zhuang, M.; **Chen, S.**; Liu, L.; Wang, N.; Gao, Z. **High-accuracy physical property prediction for pure organics via molecular representation learning: bridging data to discovery.** *npj Computational Materials*, 2025, 11, Article 224. DOI: **10.1038/s41524-025-01720-4**.
2022-11	Wang, J.; **Chen, S.**; Yang, Y.; Yu, Y.; Dong, H.; Li, Y. **Bulk structure of Si_2BN predicted by computational approaches.** *Diamond and Related Materials*, 2022, 130, 109530. DOI: **10.1016/j.diamond.2022.109530**.

Date	Citation
2021-12	Zheng, F.; Ji, Y.; Dong, H.; Liu, C.; **Chen, S.**; Li, Y. **Edge Effect Promotes Graphene-Confining Single-Atom Co-N_4 and Rh-N_4 for Bifunctional Oxygen Electrocatalysis.** *The Journal of Physical Chemistry C*, 2022, 126(1). DOI: **10.1021/acs.jpcc.1c07691**.
2021-05	**Chen, S.**; Zheng, F.; Feng, J.; Dong, H.; Li, Y. **Theoretical study on single-side fluorinated graphene for lithium storage.** *Applied Surface Science*, 2021, 560, 150033. DOI: **10.1016/j.apsusc.2021.150033**.
2017-02	Yue, L.; Pan, X.; **Chen, S.**; Song, J.; Liu, C.; Luo, G.; Guan, R.; Zhang, W. **High lithium storage capacity achieved by regulating monodisperse C/In_2O_3 nanosheet composite with double phases.** *Materials Chemistry and Physics*, 2017, 193, 89-98. DOI: **10.1016/j.matchemphys.2017.02.020**.

Patents

Publication date	Patent No.	Title	Applicant / Patent holder	Inventors / Designers
2026-03-10	**CN309838456S**	Graphical user interface for quantitative structure-activity prediction on electronic equipment	Beijing DP Technology Co., Ltd.	Jin Peng, Ji Xiaohong, **Chen Shangqian**, Cui Yaning, Wang Hongshuai, Gao Zhifeng, Zhang Linfeng, Sun Weijie
2025-09-23	**CN117327106B**	Boron-containing organic compound and organic electroluminescent device containing the same	Jiangsu Sunera Technology Co., Ltd.	**Chen Shangqian**, Zhang Fuguang, Hou Meihui, Cao Xudong
2025-05-30	**CN118206574B**	Boron-containing organic compound and organic electroluminescent device prepared from the same	Huawei Technologies Co., Ltd.; Jiangsu Sunera Technology Co., Ltd.	Cao Xudong, Zhan Ge, Wu Jiang, Liang Xiao, **Chen Shangqian**, Duan Lian
2025-04-04	**CN118084952B**	Boron-containing organic compound and organic electroluminescent device prepared from the same	Jiangsu Sunera Technology Co., Ltd.	**Chen Shangqian**, Cao Xudong, Duan Lian
2025-03-28	**CN119708023A**	Boron-containing resonance organic compound and organic electroluminescent device containing the same	Jiangsu Sunera Technology Co., Ltd.	**Chen Shangqian**
2024-06-18	**CN118206575A**	Boron-containing organic compound and organic electroluminescent device prepared from the same	Huawei Technologies Co., Ltd.; Jiangsu Sunera Technology Co., Ltd.	Cao Xudong, Liang Xiao, Zhan Ge, **Chen Shangqian**, Wu Jiang, Duan Lian
2023-06-30	**CN116354943A**	Compound containing triazine and dibenzofive-membered-ring structure and application thereof	Jiangsu Sunera Technology Co., Ltd.	**Chen Shangqian**, Sang Shenglong, Cao Xudong
2023-02-24	**CN115710265A**	Arylamine organic compound and application thereof	Jiangsu Sunera Technology Co., Ltd.	**Chen Shangqian**, Tang Dandan, Cui Ming
2019-01-08	**CN106281313B**	Silicate phosphor, preparation method, and application	Yancheng Institute of Technology	Guan Rongfeng, Zhang Jinpeng, Chi Xianhu, Shao Rong, Wang Jialiang, **Chen Shangqian**, Zhao Yuan, Li Yu
2016-11-09	**CN106077704A**	Ultra-long silver nanowire, preparation method, and application	Yancheng Institute of Technology	Guan Rongfeng, Zhang Jinpeng, Chi Xianhu, Shao Rong, Wang Jialiang, **Chen Shangqian**, Zhao Yuan, Li Yu