

宋晓壮

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教育背景

香港中文大学 (深圳)	深圳
计算机科学博士 (方向: <i>AI for Science</i> 、 <i>LLM</i> +推理与规划、数据表征学习和生成)	2023.09 – 2027.03 (预计)
南方科技大学	深圳
计算机科学与工程 硕士 (方向: 多任务学习、迁移学习、时空数据建模)	2019.09 – 2022.07
北京邮电大学	北京
数字媒体技术 工学学士	2015.09 – 2019.07

研究与实习经历

研究实习生	上海
上海人工智能实验室	2025.07 – 至今
<ul style="list-style-type: none">作为多步逆合成反应规划项目核心成员, 构建面向逆合成路线规划的端到端全栈平台, 打通模板检索、单步候选生成与多步树搜索, 接入自主搭建和集成的MoSyn指标体系实现路线规划能力落地; 研发RetroGEF: 以连续时间动态图编辑过程统一反应物图的原子增长与结构修正, 通过配对图随机桥和生成器匹配学习多种编辑顺序与原子对应关系, 更好地适配原子数变化的反应物图生成 (ICLR 2027 under review)。参与并推进Coverage Before Control (RIGS)单步逆合成工作, 将自然语言路线指令映射为候选偏好并通过轻量残差适配器引导冻结的 Graph Transformer, 实现按指定结构偏好生成前体分子。参与ChemJEPA (Latent JEPA)工作, 结合自回归学习与联合嵌入预测, 使潜在推理表征预测未来文本与分子状态, 增强化学推理与分子编辑能力 (ICLR 2027 Conference Submission)。参与MolEmb工作, 探索多模态大语言模型作为通用分子嵌入模型的能力, 支撑分子性质预测。设计了AOT*, 一个LLM引导的结构化规划与搜索框架: 利用LLM生成完整多步规划路径并映射至AND-OR树结构实现中间结果全局复用, 结合RAG检索 (364K路径库)、UCB驱动棵树搜索与奖励分配策略。设计了包含fallback模糊搜索机制的多级验证管线, 使系统在LLM输出不可靠时仍能通过语义相似性恢复有效结果。同时主导了系统工程优化: PatternFP+Tversky模板预排序使查找耗时降低57倍、Hopcroft-Karp二部图匹配将反应物验证从$O(N!)$降至$O(E\sqrt{V})$、混合多进程+多线程并行架构。在多个基准上达到SOTA, 搜索效率较现有方法提升数倍 (ACL 2026 Findings)。	
研究实习生	上海
上海人工智能实验室	2024.12 – 2025.02
<ul style="list-style-type: none">设计了ReKG-MCTS, 一个LLM + MCTS推理框架: 将LLM在结构化数据上的多步推理建模为序贯决策过程, 通过蒙特卡洛树搜索 (UCB选择、路径扩展、LLM引导的rollout、价值回传) 系统化地探索推理空间 (ACL 2025 Findings)。	
研究实习生	北京
微软亚洲研究院 (MSRA)	2021.06 – 2023.06
<ul style="list-style-type: none">在Machine Learning Area做研究型实习, mentor为Shun Zheng博士与Jiang Bian博士。提出基于元学习的多任务分组框架, 在有限训练预算下高效识别近最优任务组合方案, 在医疗序列、能源序列任务上取得可观的性能提升 (NeurIPS 2022)。参与NeurIPS 2022 CityLearn Challenge (第5名): 针对电网社区的电池充放电控制策略, 采用动态规划求解近似最优策略结合模仿学习, 赛后受邀合著优秀方案总结 (NeurIPS 2022 Competition Track)。参与表格数据表示学习项目 (ICLR 2024 Spotlight)。	

研究兴趣与技能

兴趣方向: AI For Science; LLM+结构化搜索、推理与规划; 结构化数据表示学习、应用驱动的大模型研究
技术栈: Python, PyTorch, DeepSpeed, L^AT_EX, Shell; 熟练使用Slurm等集群调度/训练工具; 目前熟练使用Claude Code、OpenAI Codex CLI等Agentic Coding工具, 具有一年以上Vibe Coding实践经验
综合能力: 在不同集群供应平台(Azure, 阿里云, 火山云等)上开展过实验, 熟悉环境配置和相关概念; 在AI工具大规模应用前有学校和公司Linux服务器管理经验; 具备良好文档自学能力与主动沟通协作能力, 上手速度较快。

其他经历

助教经历: 2023秋 DDA3020 机器学习, 2024春 CSC3150 操作系统, 2024秋 STA2001 概率与统计推断, 2025秋 CSC1001 计算机科学导论(700人大课Leading TA), 2026春 数据结构
竞赛经历: NeurIPS 2022 CityLearn Challenge 第5名, CCF-BDCI 2020 道路时空预测 前10%
专利: 硕士期间参与6项发明专利, 均已公开

审稿服务: 从2022年开始长期担任包括 NeurIPS, ICML, ICLR, WWW, AISTATS, CVPR, KDD, AAAI, ACM MM, BMVC, TPAMI, TKDE, TITS, TKDD, TII, TIP, IOTJ 等等领域内头部会议期刊审稿工作。研究成果覆盖 AI for Science、单步/多步逆合成、LLM 推理与结构化图生成等方向。

在投

- **Xiaozhuang Song**, Xuemin Chen, Xinjian Zhao, Yaoyao Xu, Tianshu Yu. *RetroGEF: Dynamic Graph Edit Flow for Single-Step Retrosynthesis*. **ICLR 2027 under review / arXiv preprint**
- Xinjian Zhao, Yaoyao Xu, Xuemin Chen, **Xiaozhuang Song**, Tianshu Yu. *Latent JEPA: Abstract Future Prediction for Latent Reasoning in Chemistry*. **ICLR 2027 Conference Submission**
- Yaoyao Xu, Xinjian Zhao, **Xiaozhuang Song**, Xuemin Chen, Tianshu Yu. *ChemOPD: Multi-Teacher On-Policy Distillation for Multi-Task Chemical Reasoning*. **ICLR 2027 Conference Submission**
- Xuemin Chen, **Xiaozhuang Song**, Xinjian Zhao, Yaoyao Xu, Tianshu Yu. *Coverage Before Control: Route-Instruction Grounding and Steering for Controllable Retrosynthesis*. **ICLR 2027 Conference Submission**
- Yaoyao Xu, Xinjian Zhao, **Xiaozhuang Song**, Lei Bai, Tianshu Yu. *Closed-Loop Bayesian Molecular Inverse Design with Semantic LLM Surrogates*. **arXiv:2608.22967**, 2026.

已接收/发表

- **Xiaozhuang Song**, Xuanhao Pan, Xinjian Zhao, Hangting Ye, Shufei Zhang, Jian Tang, Tianshu Yu. *AOT*: Efficient Synthesis Planning via LLM-Empowered AND-OR Tree Search*. **ACL 2026 Findings**
- **Xiaozhuang Song**, Shufei Zhang, Tianshu Yu. *ReKG-MCTS: Reinforcing LLM Reasoning on KGs via Training-Free MCTS*. **ACL 2025 Findings**
- **Xiaozhuang Song**, Tianshu Yu. *Physically-Informed Flow Matching with Graph Neural Networks for Complex Fluid Dynamics*. **AAAI 2026 [CCF-A]**
- **Xiaozhuang Song**, Yuzhao Tu, Hangting Ye, Wei Fan, Qingquan Zhang, Xiaoxue Wang, Tianshu Yu. *Enhancing Generalizability in Molecular Conformation Generation with Metrization-Informed Geometric Diffusion Pretraining*. **AAAI 2025 [CCF-A]**
- **Xiaozhuang Song**, Shun Zheng, Wei Cao, James J.Q. Yu, Jiang Bian. *Efficient and Effective Multi-task Grouping via Meta Learning on Task Combinations*. **NeurIPS 2022 [CCF-A]**
- **Xiaozhuang Song**, Yuzhao Tu, Tianshu Yu. *Enhancing Molecular Conformer Generation via Fragment-Augmented Diffusion Pretraining*. **TMLR 2025**
- **Xiaozhuang Song**, Xu Liao, Hangting Ye, Yaoyao Xu, Wei Fan, Jin Liu, Tianshu Yu. *Single Cell Gene Expression Prediction via Prototype-based Proximal Neural Factorization*. **BIBM 2024 [CCF-B]**
- **Xiaozhuang Song**, Ying Wu, Chenhan Zhang. *TSTNet: A Seq2Seq Transformer for Spatial-temporal Traffic Prediction*. **ICANN 2021 [CCF-C]**
- Hangting Ye, Peng Wang, Wei Fan, **Xiaozhuang Song**, He Zhao, Dandan Guo, Yi Chang. *Deep Tabular Representation Corrector*. **TPAMI 2026 [CCF-A]**
- Xinjian Zhao, Wei Pang, Zhixuan Yu, Xiangru Jian, **Xiaozhuang Song**, Yaoyao Xu, Zhongkai Xue, Dingshuo Chen, Shu Wu, Philip Torr, Tianshu Yu. *When Vision Meets Graphs: A Survey on Graph Reasoning and Learning*. **IJCAI 2026 (Survey Track)**
- Xinjian Zhao, Xiangru Jian, Yaoyao Xu, **Xiaozhuang Song**, Wei Pang, Lei Bai, Tianshu Yu. *MolEmb: Multimodal Large Language Models Can Be Strong Molecular Embedding Models*. **ICML 2026 Workshop (FM4LS)**
- Xinjian Zhao, Wei Pang, Zhongkai Xue, Xiangru Jian, Lei Zhang, Yaoyao Xu, **Xiaozhuang Song**, Shu Wu, Tianshu Yu. *The Underappreciated Power of Vision Models for Graph Structural Understanding*. **NeurIPS 2025 [CCF-A]**
- Wei Fan, Jingru Fei, Dingyu Guo, Kun Yi, **Xiaozhuang Song**, Haolong Xiang, Hangting Ye, Min Li. *MedGNN: Multi-resolution Spatiotemporal Graph Learning for Medical Time Series*. **WWW 2025 [CCF-A]**
- Hangting Ye, Wei Fan, **Xiaozhuang Song**, Shun Zheng, He Zhao, Dandan Guo, Yi Chang. *PTaRL: Prototype-based Tabular Representation Learning*. **ICLR 2024 Spotlight [CCF-A]**
- Wei Fan, Jingru Fei, Junwen Han, Jinglan Lian, Hangting Ye, **Xiaozhuang Song**, Xiaoling Lv, Kun Yi, Min Li. *Medvia: Medical Time Series Classification with Vision Augmentation*. **Information Fusion 2025 [JCR Q1, IF 14.7]**
- Yunjie Huang, **Xiaozhuang Song**, Shiyao Zhang, Lei Li, James J.Q. Yu. *GT-TTE: Modeling Trajectories as Graphs for Travel Time Estimation*. **IEEE IoT Journal 2024 [JCR Q1]**

- Yunjie Huang, **Xiaozhuang Song**, Yuanshao Zhu, Shiyao Zhang, James J.Q. Yu. *Traffic Prediction with Transfer Learning*. **IEEE T-ITS 2023 [CCF-B / JCR Q1]**
- Ao Wang, Yongchao Ye, **Xiaozhuang Song**, Shiyao Zhang, James J.Q. Yu. *Traffic Prediction With Missing Data*. **IEEE T-ITS 2023 [CCF-B / JCR Q1]**
- Yaoyao Xu, Xinjian Zhao, **Xiaozhuang Song**, Benyou Wang, Tianshu Yu. *Boosting Protein Language Models with Negative Sample Mining*. **ECML-PKDD 2024 [CCF-B]**
- Kingsley Nweye, ..., **Xiaozhuang Song**, ..., Shun Zheng, Jiang Bian. *The CityLearn Challenge 2022*. **NeurIPS 2022** Competition Track
- Yunjie Huang, **Xiaozhuang Song**, Shiyao Zhang, James J.Q. Yu. *Transfer Learning in Traffic Prediction with GNNs*. **IEEE ITSC 2021**
- **Xiaozhuang Song**, Christos Markos, James J.Q. Yu. *Multimix: Multi-task Deep Learning for Travel Mode Identification*. **IEEE ITSC 2020**