Wenjie Du

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籍贯：河南省济源市
出生年月：1996.04
政治面貌：党员

教育经历

- 2014 年-2018 年，东北大学，冶金学院，环境科学，本科/学士，王梅
- 2018 年-2021 年，中国科学技术大学， 应用化学系，硕士，李文卫
- 2021 年-2023 年，中国科学技术大学，软件学院，博士，汪炀

主要获奖

- 2021 年姑苏特等奖学金
- 2022 年中国科学技术大学“深交所”奖学金
- 2023 年北京大学唐孝炎奖学金
- 2023 年中科院院长奖学金
- 2023 年中国科学技术大学“深交所”奖学金

研究方向

- **知识与数据驱动的 AI for Science 研究：**

  1）AI 与环境的结合

  运用神经网络、知识图谱、迁移学习等先进人工智能算法模型，预测水质或者空气质量，并基于预测结果给出响应控制策略；碳排放计算。

  2）AI 与化学的结合

  着力实现对构象异构体和手性分子的区分以及相应的化学性质预测。

  3）AI 与材料分子的结合

  着力解决材料吸附过程中的溶剂化效应；以及通过解读光谱还原催化过程。

参与课题

[1] 中国科学院基础研究领域优秀青年团队（人工智能大数据与化学、材料或生物科学的结合），No.YSBR-005, 2021-2024；

[2] 国家重大科研仪器设备研制专项，面向红外芯片的光谱与界面功能关系研究的多尺度表征系统，2023.01-2027.12；

代表作 **（除标注 submitted 外其余均已被接收）：**

AI for science **（一作或共同一作成果）:**

[1] **Wenjie Du**, JiaYuan Lu, YiRong Hu, Juanxiu Xiao, Jie Wu, Cheng Yang, Baocheng Huang, Shuo Cui, Yang Wang, Wenwei Li, Spatiotemporal Pattern of Greenhouse Gas Emissions in China’s Wastewater Sector and Pathways towards Carbon Neutrality. ***Nature Water,2023***.

[2] **Wenjie Du**, Fenfen Ma, Jiahui Zhang, Baicheng Zhang, Xiaoting Yang, Wu Di, Yang Wang,

and Jun Jiang, Spectroscopy-Guided Deep Learning Predicts Solid-Liquid Surface Adsorbate Properties in Unseen Solvents. ***Journal of the American Chemical Society. (JACS*** **化学领域顶刊, 中科院一区， IF = 15. 419)**

[3] **Wenjie Du**, Shuai Zhang, Ziyuan Zhao, Jun Xia, Junfeng Fang, Yang Wang, MMGNN: A Molecular Merged Graph Neural Network for Explainable Solvation Free Energy Prediction. ***the 33rd International Joint Conference on Artificial Intelligence*** (**CCF A**).

[4] **Wenjie Du**, Xiaoting Yang, Di Wu, FenFen Ma, Baicheng Zhang, Chaochao Bao, Yaoyuan Huo, Xin Chen, **Yang Wang***. Fusing 2D and 3D Molecular Graphs as Unambiguous Molecular Descriptors for Conformational and Chiral Stereoisomers. ***Briefings in Bioinformatics,2023***. (JCR Q1, IF= 13.994, CCF B)

[5] **Wenjie Du**, Lianliang Chen, Haoran Wang, Ziyang Shan, Zhengyang Zhou, Wenwei Li, Yang Wang*, Deciphering Urban Traffic Impacts on Air Quality by Deep Learning and Emission Inventory. ***Journal of Environmental Sciences,2023***. (JCR Q1, IF= 6.796, **高被引论文**)

[6] Yirong Hu, **Wenjie Du**, Cheng Yang, **Yang Wang***, Tianyin Huang, Xiaoyi Xu, Wenwei Li*. Source identification and prediction of nitrogen and phosphorus of Lake Taihu by ensemble Machine Learning Technique, ***Frontiers of Environmental Science & Engineering,2023***. (JCR Q2, IF= 6.048)

[7] Baicheng Zhang, Xiaolong Zhang, **Wenjie Du**, Zhaokun Song, Guozhen Zhang, Guoqing Zhang, **Yang Wang**, Xin Chen, Jun Jiang, and Yi Luo, Chemistry-informed molecular graph as reaction descriptor for machine-learned retrosynthesis planning. ***Proceedings of the National Academy of Sciences (PNAS),2022***.（**美国科学院院刊，中科院一区， IF = 11.1**）

AI for science **(通讯作者成果)**:

[8] Xin Meng, Binglan Wu, Yilei Liang, Chenkai Gu, **Wenjie Du#,** Xin Chen#, CIMG-BERT: pretraining bidirectional transformers with chemistry knowledge for molecular property prediction. ***IEEE International Conference on Information Technology, Communication Ecosystem and Management,2022.*** (EI)

[9] Jiahui Zhang, **Wenjie Du*,#**, Binglan Gu, Xiaoting Yang, Xin Chen, Yang Wang#, SMG-BERT: integrating stereoscopic information and chemical representation for molecular property prediction. ***Frontiers In Molecular Biosciences*** (JCR Q1, IF= 6.133)

[10] Jiahui Zhang*, **Wenjie Du*, #**, Di Wu, Jiahe Li, Shuai Zhang, Yang Wang#, Improving efficiency in rationale discovery for Out-of-Distribution molecular representations. ***International Conference on Bioinformatics and Biomedicine (BIBM)*** (CCF B)

[11] Jiahe Li*, **Wenjie Du*, #**, Di Wu, Jiahui Zhang, Shuai Zhang, Yang Wang#, MolCLW: Molecular Contrastive Learning with Learnable Weighted Subgraph Structure. ***Briefings in Bioinformatics (submitted)***

[12] Shuai Zhang*, **Wenjie Du*, #**, Di Wu, Jiahe Li, Jiahui Zhang, Yang Wang#, AI-DDI: An Attention-Based Substructure Interactive Model for Predicting Drug-Drug Interaction. ***Briefings in Bioinformatics (submitted)***

AI for science **(非一作成果)**:

[13] Ziyang Shan, **Wenjie Du,** Correlation between Nitrogen Pollution and WWTPs Discharge in Lake Taihu. ***3rd International Conference on Advances in Computer Technology, Information Science and Communication (CTISC),2021.*** (EI)

[14] Jingxiao Zhang, Tian Tian, **Wenjie Du,** Yanfan Guan, Yunjie Wang, Yusheng Li, Hanqing Yu. Adopting vibration to alleviate the solute buildup and membrane fouling in a forward osmosis system. ***Journal of Cleaner Production,2021.*** (JCR Q1, IF= 11.072)

[15] Cheng Yang, **Wenjie Du,** Ruli He, Yirong Hu, Houqi Liu, Tianyin Huang, Wenwei Li. Spatiotemporal patterns of methane and nitrous oxide emissions in China's inland waters predicted by machine learning technique. ***ACS ES&T Water*** (JCR Q1,)**.**

[16] Xiaoting Yang, **Wenjie Du**, Bond Energy Assists Accurate Molecule Property Prediction.

Journal of Physics: Conference Series (EI)

[17] Yifan Xie, Shou Feng, LinXiao Deng, Aoran Cai, Liyu Gan, Zifan Jiang, Peng Yang, Guilin Ye, Zaiqing Liu, Li Wen, Qing Zhu, Wanjun Zhang, Zhanpeng Zhang, Jiahe Li, Zeyu Feng, Chutian Zhang, **Wenjie Du**, Lixin Xu, Jun Jiang, Xin Chen, Gang Zou. Inverse design of chiral functional filme by a robotic AI-Chemist. ***Nature Communication***. (JCR Q1, IF= 17.694)

专利与软件著作：

[18] 金美伶，**杜文杰**，王梅，杨合，纪肇烨；一种有优良抗菌性能的抗菌陶瓷的制备方法。CN201811009336.9 (发明专利)

[19] 汪炀，**杜文杰**，杨笑听，吴迪，李家和；分子性质及合成路径预测软件。(软件著作权)