# Yuqi Song

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## EDUCATION

**University of South Carolina** — Columbia, SC
*PhD in Computer Science* — *Aug 2019 - Aug 2023*
Supervised by *Dr. Jianjun Hu*
**Dissertation Title:** *Predicting Material Structures and Properties Using Deep Learning and Machine Learning Algorithms*

**Chongqing University** — Chongqing, China
*Master in Software Engineering* — *Sept 2016 - Jun 2019*

**Chongqing University** — Chongqing, China
*Bachelor in Software Engineering* — *Sept 2012 - Jun 2016*

## TEACHING EXPERIENCE

- COS 470 Introduction of Artificial Intelligence, Fall 2023, University of Southern Maine

- COS 160 Structured Problem Solving using Java, Fall 2023, University of Southern Maine

- Instructional Assistant, Algorithmic Design II, Spring 2023, University of South Carolina

- Instructional Assistant, Algorithmic Design I, Fall 2021, Spring 2022, Fall 2022, University of South Carolina

- Teaching Assistant, Programming Language Structures, Fall 2019, University of South Carolina

## PUBLICATIONS

**Journal Articles (Peer-Reviewed)**

[1] Jianjun Hu, Yong Zhao, Qin Li, **Yuqi Song**, Rongzhi Dong, Wenhui Yang, and Edirisuriya MD Siriwardane. "Deep Learning-Based Prediction of Contact Maps and Crystal Structures of Inorganic Materials". In: *ACS Omega* (2023).

[2] Nihang Fu, Lai Wei, **Yuqi Song**, Qinyang Li, Rui Xin, Sadman Sadeed Omee, Rongzhi Dong, Edirisuriya M Dilanga Siriwardane, and Jianjun Hu. "Material transformers: deep learning language models for generative materials design". In: *Machine Learning: Science and Technology* 4.1 (2023), p. 015001.

[3] Jeffrey Hu and **Yuqi Song**. "Piezoelectric modulus prediction using machine learning and graph neural networks". In: *Chemical Physics Letters* 791 (2022), p. 139359.

[4] Rongzhi Dong, Yong Zhao, **Yuqi Song**, Nihang Fu, Sadman Sadeed Omee, Sourin Dey, Qinyang Li, Lai Wei, and Jianjun Hu. "DeepXRD, a Deep Learning Model for Predicting of XRD spectrum from Materials Composition". In: *ACS Applied Materials & Interfaces* 14.35 (2022), pp. 40102–40115.

[5] Jianjun Hu, Stan Stef, **Yuqi Song**, Sadman Sadeed Omee, Steph-Yves Louis, Edirisuriya Siriwardane, Yong Zhao, and Lai Wei. "MaterialsAtlas. org: a materials informatics web app platform for materials discovery and survey of state-of-the-art". In: *npj Computational Materials* 8.1 (2022), pp. 1–12.

[6] Feng Jiang, Yang Cao, Huan Wu, Xibin Wang, **Yuqi Song**, and Min Gao. "Social Recommendation Based on Multi-Auxiliary Information Constrastive Learning". In: *Mathematics* 10.21 (2022), p. 4130.

[7] **Yuqi Song**, Edirisuriya M Dilanga Siriwardane, Yong Zhao, and Jianjun Hu. "Computational discovery of new 2D materials using deep learning generative models". In: *ACS Applied Materials & Interfaces* 13.45 (2021), pp. 53303–53313.

[8] Yong Zhao, Mohammed Al-Fahdi, Ming Hu, Edirisuriya MD Siriwardane, **Yuqi Song**, Alireza Nasiri, and Jianjun Hu. "High-throughput discovery of novel cubic crystal materials using deep generative neural networks". In: *Advanced Science* 8.20 (2021), p. 2100566.

[9] Rui Xin, Edirisuriya MD Siriwardane, **Yuqi Song**, Yong Zhao, Steph-Yves Louis, Alireza Nasiri, and Jianjun Hu. "Active-Learning-Based Generative Design for the Discovery of Wide-Band-Gap Materials". In: *The Journal of Physical Chemistry C* 125.29 (2021), pp. 16118–16128.

[10] **Yuqi Song**, Joseph Lindsay, Yong Zhao, Alireza Nasiri, Steph-Yves Louis, Jie Ling, Ming Hu, and Jianjun Hu. "Machine learning based prediction of noncentrosymmetric crystal materials". In: *Computational Materials Science* 183 (2020), p. 109792.

[11] Steph-Yves Louis, Yong Zhao, Alireza Nasiri, Xiran Wang, **Yuqi Song**, Fei Liu, and Jianjun Hu. "Graph convolutional neural networks with global attention for improved materials property prediction". In: *Physical Chemistry Chemical Physics* 22.32 (2020), pp. 18141–18148.

[12] Xiang Li, Yabo Dan, Rongzhi Dong, Zhuo Cao, Chengcheng Niu, **Yuqi Song**, Shaobo Li, and Jianjun Hu. "Computational screening of new perovskite materials using transfer learning and deep learning". In: *Applied Sciences* 9.24 (2019), p. 5510.

[13] Junliang Yu, Min Gao, Wenge Rong, **Yuqi Song**, and Qingyu Xiong. "A social recommender based on factorization and distance metric learning". In: *IEEE Access* 5 (2017), pp. 21557–21566.

## Conference and Workshop Papers

[1] Xin Zhang, Rabab Abdelfattah, **Yuqi Song**, Samuel A Dauchert, and Xiaofeng Wang. "Depth Monocular Estimation with Attention-based Encoder-Decoder Network from Single Image". In: *2022 IEEE 24th Int Conf on High Performance Computing & Communications; 8th Int Conf on Data Science & Systems; 20th Int Conf on Smart City; 8th Int Conf on Dependability in Sensor, Cloud & Big Data Systems & Application (HPCC/DSS/SmartCity/DependSys)*. IEEE. 2022, pp. 1795–1800.

[2] Xin Zhang, Rabab Abdelfattah, **Yuqi Song**, and Xiaofeng Wang. "An Effective Approach for Multi-label Classification with Missing Labels". In: *2022 IEEE 24th Int Conf on High Performance Computing & Communications; 8th Int Conf on Data Science & Systems; 20th Int Conf on Smart City; 8th Int Conf on Dependability in Sensor, Cloud & Big Data Systems & Application (HPCC/DSS/SmartCity/DependSys)*. IEEE. 2022, pp. 1713–1720.

[3] Xin Zhang, Hong Xiang, and **Yuqi Song**. "Meta-path and matrix factorization based shilling detection for collaborate filtering". In: *Collaborative Computing: Networking, Applications and Worksharing: 14th EAI International Conference, CollaborateCom 2018, Shanghai, China, December 1-3, 2018, Proceedings 14*. Springer. 2019, pp. 3–16.

[4] Junwei Zhang, Min Gao, Junliang Yu, Xinyi Wang, **Yuqi Song**, and Qingyu Xiong. "Nonlinear Transformation for Multiple Auxiliary Information in Music Recommendation". In: *2019 International Joint Conference on Neural Networks (IJCNN)*. IEEE. 2019, pp. 1–8.

[5] **Yuqi Song**, Min Gao, Junliang Yu, and Qingyu Xiong. "Social recommendation based on implicit friends discovering via meta-path". In: *2018 IEEE 30th International Conference on Tools with Artificial Intelligence (ICTAI)*. IEEE. 2018, pp. 197–204.

[6] Fan Yang, Min Gao, Junliang Yu, **Yuqi Song**, and Xinyi Wang. "Detection of shilling attack based on bayesian model and user embedding". In: *2018 IEEE 30th International Conference on Tools with Artificial Intelligence (ICTAI)*. IEEE. 2018, pp. 639–646.

[7] **Yuqi Song**, Min Gao, Junliang Yu, Wentao Li, Lulan Yu, and Xinyu Xiao. "PUED: A Social Spammer Detection Method Based on PU Learning and Ensemble Learning". In: *Collaborative Computing: Networking, Applications and Worksharing: 13th International Conference, CollaborateCom 2017, Edinburgh, UK, December 11–13, 2017, Proceedings 13*. Springer. 2018, pp. 143–152.

[8] Zehua Zhao, Min Gao, Junliang Yu, **Yuqi Song**, Xinyi Wang, and Min Zhang. "Impact of the important users on social recommendation system". In: *Collaborative Computing: Networking, Applications and Worksharing: 13th International Conference, CollaborateCom 2017, Edinburgh, UK, December 11–13, 2017, Proceedings 13*. Springer. 2018, pp. 425–434.

[9] Tong Dou, Junliang Yu, Qingyu Xiong, Min Gao, **Yuqi Song**, and Qianqi Fang. "Collaborative shilling detection bridging factorization and user embedding". In: *Collaborative Computing: Networking, Applications and Worksharing: 13th International Conference, CollaborateCom 2017, Edinburgh, UK, December 11–13, 2017, Proceedings 13*. Springer. 2018, pp. 459–469.

[10] Junliang Yu, Min Gao, **Yuqi Song**, Zehua Zhao, Wenge Rong, and Qingyu Xiong. "Connecting factorization and distance metric learning for social recommendations". In: *Knowledge Science, Engineering and Management: 10th International Conference, KSEM 2017, Melbourne, VIC, Australia, August 19-20, 2017, Proceedings 10*. Springer. 2017, pp. 389–396.

[11] Junliang Yu, Min Gao, Wenge Rong, **Yuqi Song**, Qianqi Fang, and Qingyu Xiong. "Make users and preferred items closer: Recommendation via distance metric learning". In: *Neural Information Processing: 24th International Conference, ICONIP 2017, Guangzhou, China, November 14–18, 2017, Proceedings, Part V 24*. Springer. 2017, pp. 297–305.

## Preprints and In Preparation

[1] Xin Zhang, **Yuqi, Song**, Xiaofeng Wang, and Fei Zuo. "D-Score: A White-Box Diagnosis Score for CNNs Based on Mutation Operators". In: *arXiv preprint arXiv:2304.00697* (2023).

[2] Rongzhi Dong, **Yuqi, Song**, Edirisuriya Siriwardane, and Jianjun Hu. "Discovery of 2D materials using Transformer Network based Generative Design". In: *arXiv preprint arXiv:2301.05824* (2023).

[3] Lai Wei, Nihang Fu, **Yuqi, Song**, Qian Wang, and Jianjun Hu. "Probabilistic Generative Transformer Language models for Generative Design of Molecules". In: *arXiv preprint arXiv:2209.09406* (2022).

[4] Lai Wei, Qinyang Li, **Yuqi, Song**, Stanislav Stefanov, Edirisuriya Siriwardane, Fanglin Chen, and Jianjun Hu. "Crystal transformer: Self-learning neural language model for generative and tinkering design of materials". In: *arXiv preprint arXiv:2204.11953* (2022).