Department of Computer Science
香港城市大學
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**COMPUTER SCIENCE COLLOQUIUM**

# Material Network Science as A New Paradigm For Matter Design


SPEAKER **Dr. Yuan-chao HU**

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VENUE Y5302, 5th Floor, Yellow Zone, Yeung Kin Man Academic Building, City University of Hong Kong, 83 Tat Chee Avenue, Kowloon Tong

## ABSTRACT


The space of possible materials is vast, bounded only by the combinatorial possibilities of chemical elements and their compositions. This renders grand challenges in designing functional materials with desired properties. To accelerate this process, we propose a material network science paradigm with data-driven learning strategies. By accumulating various data, we construct network representations to predict unresolved material properties, such as the glass-forming ability and soft-magnetic properties of metallic glasses, and phase formation in high-entropy alloys. We then employ sophisticated graph mining and deep learning to uncover hidden relationships within these material networks. This motivates a material recommendation system empowered by graph neural networks and natural language processing-derived elemental embeddings. We extend to learning comprehensive encodings of chemical elements by network representations and language mining, laying the foundation for AI-driven material design. The AI-assisted material network science paves a new way for the intelligent and efficient navigation of material space.


## BIOGRAPHY

Dr. Yuan-chao Hu, principle investigator leading the data-driven materials science research group at Songshan Lake Materials Laboratory (SLAB). Dr. Hu earned his Ph.D.s from Institute of Physics, Chinese Academy of Science, and City University of Hong Kong in 2018. After graduation, Dr. Hu was trained at Yale University as Postdoctoral Research Associate and Associate Research Scientist, and at The University of Tokyo as JSPS Postdoctoral Fellow. Dr. Hu has been engaged in computational materials science and physics for more than 10 years, specifically in computer simulations of disordered systems. Over the last decade, Dr. Hu published more than 40 peer-reviewed journal publications in National Science Review, Nature Materials, Nature Energy, Nature Physics, Nature Communications, Science Advances, PNAS, Advanced Materials etc. Currently, Dr. Hu focuses on both computational materials sceince and "AI+Materials", and serves as Associate Editor for "Science China Physics, Mechanics & Astronomy" and Executive Editor for "AI for Science".

**All are welcome!**

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