



Department of  
Mechanical Engineering  
The University of Hong Kong



Tam Wing Fan  
Inno Wing Two

FACULTY OF ENGINEERING

## SEMINAR

### Domain Knowledge-Guided Materials AI Experiments and Computations

**Date:** 19 October, 2023 (Thursday)  
**Time:** 2:30 p.m.  
**Venue:** Tam Wing Fan Innovation Wing Two  
G/F, Run Run Shaw Building, HKU

**Speaker:** Prof. Tong-Yi Zhang  
Founding Dean of Materials Genome Institute  
Shanghai University



**Moderator:** Prof. David Srolovitz  
Professor of Mechanical Engineering, Chair of Materials Theory  
The University of Hong Kong

#### Abstract:

This presentation briefly introduces the concept of Materials Informatics and Materials-GPT. Materials informatics is growing extremely fast by integrating Artificial Intelligence (AI) and machine learning with materials science and engineering to accelerate materials science, engineering and manufacturing innovations. Particularly, the birth of Chat-GPT-4 further pours oil on the flames of Materials Informatics and hastens the parturition of Materials-GPT. Two fundamentals are there in Materials-GPT, including materials AI robots and AI labs, and materials AI computations and AI software and the both “hard” and “soft” fundamentals must be very strong and developed under the guidance of domain knowledge, which will result in materials large multimodal model. The domain knowledge-guided machine learning strategy is the best way to create new knowledge, innovate and progress materials science and engineering, and speed up the materials manufacturing. Case studies are given on the oxidation behaviours of ferritic-martensitic steels in supercritical water and the oxidation behaviours of FeCrAlCoNi based high entropy alloys at high temperature. This strategy leads to the development of formulas with high generalization and accurate prediction power, which are most desirable to science, technology, and engineering.

**Biography:**

Prof. Tong-Yi Zhang is the founding dean of Materials Genome Institute, Shanghai University, and the founding director of the Materials Genome Engineering division in the Chinese Materials Research Society (CMRS). Currently he is doing his best to promote Materials Genome Engineering and Materials/Mechanics Informatics, especially, materials AI labs, materials AI computations, and materials large multimodal model. He joined the Hong Kong University of Science and Technology (Guangzhou) in 2022. He is the founding Editor-in-Chief of Journal of Materials Informatics and was the Editor-in-Chief of Science China Technological Sciences 2018-2022. He received the awards including the 2018 Prize for Scientific and Technological Progress from the HLHL Foundation, the Second Prizes of 2007 and 1987 State Natural Science Award, China, and the 1988 National Award for Young Scientists, China. He became Fellow of International Congress on Fracture in 2013, Fellow of the Hong Kong Academy of Engineering Sciences in 2012, Member of Chinese Academy of Sciences in 2011, Senior Research Fellow of Croucher Foundation, Hong Kong, in 2003, Fellow of ASM International, USA, in 2001.

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