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# TMS 2023

## 152<sup>nd</sup> Annual Meeting & Exhibition

MARCH 19–23, 2023  
SAN DIEGO CONVENTION CENTER &  
HILTON SAN DIEGO BAYFRONT  
SAN DIEGO, CALIFORNIA, USA  
#TMSANNUALMEETING



## SUBMIT AN ABSTRACT BY JULY 1 AND JOIN US AT TMS2023 FOR THIS SPECIAL SYMPOSIUM!

### HONORARY SYMPOSIUM

## Materials Genome, CALPHAD, and a Career over the Span of 20, 50, and 60 Years: An FMD Symposium in Honor of Zi-Kui Liu

#### ABOUT THE SYMPOSIUM

This symposium is to celebrate the impact of Zi-Kui Liu on the fields of computational materials science and materials design on the occasion of his 60th birthday, the 20th anniversary of Liu coining the term "Materials Genome," and the progress of computational thermodynamics (CALPHAD) in the last 50 years as the foundation of materials design.

To honor the range of Liu's research on metals, ceramics, battery materials, and 2D materials, the symposium will highlight work that integrates theory with computational and experimental investigations and that uses a multidisciplinary approach. The symposium will focus on thermodynamics with internal processes in terms of theory, prediction, modeling, and applications. This symposium welcomes contributions including but not limited to the following topics:

- Theory of reversible and irreversible thermodynamics
- Development of computational tools for thermodynamics
- Determination of thermodynamic properties through density functional theory, machine learning models, ab initio molecular dynamic simulations, and experiments
- Thermodynamic modeling through the CALPHAD method and statistical mechanics
- Applications of thermodynamics for rational and inverse design of chemistry and synthesis of materials, simulation of kinetic processes and deformation, and understanding of complex phenomena.



#### ABOUT THE HONOREE

**Zi-Kui Liu** is the Dorothy Pate Enright professor in the Department of Materials Science and Engineering at The Pennsylvania State University. He obtained his B.S. from Central South University (China), M.S. from University of Science and Technology Beijing (China), and Ph.D. from Royal Institute of Technology (KTH, Sweden). He was a research associate at

University of Wisconsin-Madison and a senior research

scientist at Questek Innovation, LLC. He has been at the Pennsylvania State University since 1999, the editor-in-chief of *CALPHAD* journal since 2001, and the president of CALPHAD, Inc. since 2013. He co-founded the U.S. National Science Foundation Center for Computational Materials Design and served as its director from 2005 to 2014.

Liu is a Fellow of TMS and ASM International. He served as a member of the TMS Board of Directors, as the president of ASM International, and as a member of the ASM International Board of Trustees. He received the TMS William Hume-Rothery Award, the ASM J. Willard Gibbs Phase Equilibria Award, the American Ceramic Society Spriggs Phase Equilibria Award, the Wilson Award for Excellence in Research from the Pennsylvania State University, and the Lee Hsun Award from the Institute of Metals Research, Chinese Academy of Science. Liu's current research activities are centered on first-principles calculations, machine learning, modeling of thermodynamic, kinetic, and other properties including statistical mechanics and their integration for understanding defects, phase stability, and phase transformations, and designing and tailoring materials processing and properties.

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