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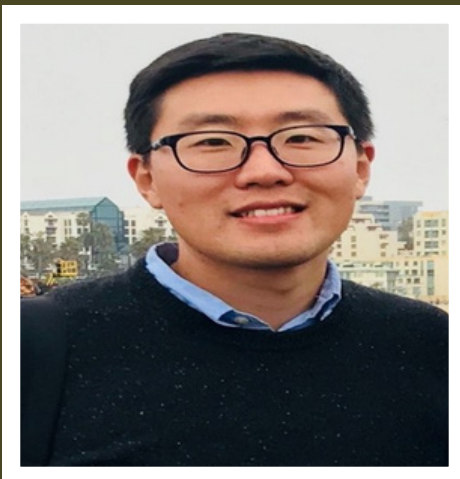
Webinar-40

Asian Consortium on Computational Materials Science (ACCMS) Global Centre

SRM University-AP, Amaravati

May 29, 2026 | 11:00 AM - 01:00 PM (IST)

AI Physics and Materials Design



Moderator

Dr Jung-Hoon Lee

Principal Research Scientist
Computational Science
Research Centre
Korea Institute of Science and
Technology (KIST)



Speaker

Prof. Xin-gao Gong

Key laboratory for computational
physics (Fudan University), MOE
AI center for physical sciences
(Fudan University), Shanghai
Education Commission),
Shanghai Education Commission

Short Biography

PXin-Gao Gong is an Academician of the Chinese Academy of Sciences (elected 2017), Xie Xide Distinguished Professor of Physics at Fudan University, and Chancellor of Guangdong Israel Institute of Technology (GDIIT). He is also a Fellow of the American Physical Society.

Professor Gong received his B.Sc. from Hunan Normal University (1982) and his Ph.D. from the Institute of Solid-State Physics, Chinese Academy of Sciences (1993). He was a Research Fellow at the International School for Advanced Studies (SISSA), Italy, from 1988 to 1991, and has held visiting professorships at Ohio State University, Clark Atlanta University, and the Chinese University of Hong Kong. He joined Fudan University in 2000 and has served in several leadership roles, including Dean of Research and Director of the Key Laboratory for Computational Physical Sciences (MOE) since 2009. His research focuses on AI-driven physics, computational design of energy materials, thermal transport, multiscale modeling methods, and interface properties. He has published over 350 papers in leading journals such as Physical Review Letters, Nature Communications, Nature Machine Intelligence, and Journal of the American Chemical Society. He is recognised as a Clarivate Highly Cited Scientist. Professor Gong has received numerous honors, including the National Natural Science Award (2nd Prize, 2012), the First-Rank Award for Natural Science from Shanghai Municipality (2009) and the Ministry of Education (2014), and the Shanghai Meritorious Statesman for Education Award (2023). He currently serves as a Representative of the 14th National People's Congress of China.

Abstract

Artificial intelligence has profoundly altered the development of the economy and society and revolutionised the paradigms of scientific research. In this talk, I will explore the impact of artificial intelligence on contemporary physics starting from the main bottlenecks of computational materials. Based on our own research, I will introduce the latest progress in molecular dynamics methods and first-principles electronic structure calculations, especially the successfully constructed universal Kohn-Sham Hamiltonian, and demonstrate how AI is changing the landscape of computational physics. Several examples will be presented to illustrate the efficiency and effectiveness of AI-based algorithms, especially in the field of material design.

Convener:

Prof. Yoshiyuki Kawazoe,
Head, ACCMS-Centre
Prof. G P Das, TCG Crest
Prof. Ranjit Thapa, SRM University-AP

Local Organisers:

Dr Mahesh Kumar Ravva,
SRM University-AP
Prof. Umesh Waghmare, JNCASR
Dr Surya VJ, ACCMS

Zoom Meeting Link:

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