



HKUST Industry Engagement Day + Digital and AI-Driven Materials Innovation

Tuesday, 8 July 2025
09:30–17:30



Padma and Hari Harilela Lecture Theater (LT-C),
HKUST Clear Water Bay Campus

Event Program

Time	Program
09:30-10:00	Guest Registration
10:00-10:05	Welcome Remarks Prof. Tim CHENG, Vice-President of Research and Development, HKUST
10:05-10:10	Opening Remarks Prof Jianzhen YU, Head and Chair Professor, Department of Chemistry, HKUST
10:10-10:15	Opening Remarks Dr. Michael RAUCH, Associate Director of Materials Science, Schrödinger Inc.
10:15-10:20	Photo-taking Session
Session Chair: Prof. Zhenyang LIN, Chair Professor of Department of Chemistry, HKUST	
10:20-10:40	Topic: Physics-Enabled AI for Next-Generation Materials Discovery: Bridging Atomic-Scale Simulation and Machine Learning with Schrödinger Dr. Michael RAUCH, Associate Director of Materials Science, Schrödinger Inc.
10:40-11:10	Topic: Materials Design in Electronics Industry: Application of Materials Informatics and High-Throughput Calculations Dr. Nobuyuki N. MATSUZAWA, Director, Panasonic Corporation
11:10-11:30	Topic: Designing Tomorrow's Materials: The Role of AI in Exchange-Correlation Functional Prof. Guanhua CHEN, Chair Professor, Department of Chemistry, HKU
11:30-14:00	Lunch
Session Chair: Prof. Kevin Jing CHEN, Chair Professor, Department of Electronic and Computer Engineering, HKUST	
14:00-14:20	Topic: AI in semiconductor industry Dr Ziyang GAO, Senior director, Hong Kong Microelectronics Research and Development Institute
14:20-14:40	Topic: Simulations of atomic level processing with examples from metal ALD Dr. Simon ELLIOTT, Senior Research Leader, Schrödinger Inc.
14:40-15:00	Topic: AI-Enabled OLED Materials Discovery Dr Wei XU, Research scientist, TCL AI Lab



HKUST Industry Engagement Day + Digital and AI-Driven Materials Innovation

Tuesday, 8 July 2025
09:30–17:30



Padma and Hari Harilela Lecture Theater (LT-C),
HKUST Clear Water Bay Campus

Event Program

Time	Program
15:00-15:20	Coffee Break
Session Chair: Prof. Ping GAO, Professor of Department of Chemical and Biological Engineering, HKUST	
15:20-15:40	<i>Topic: AI-Guided Interfacial Engineering for Rational Design of Polymeric Microcapsules</i> Prof. Jinglei YANG, Professor, Department of Mechanical and Aerospace Engineering, HKUST
15:40-16:00	<i>Topic: Advancing Specialty Polymer Innovation Using Molecular Simulation and Machine Learning</i> Dr. Atif AFZAL, Principal Scientist, Schrödinger Inc.
16:00-16:20	<i>Topic: Accelerating Pharmaceutical Formulations using the Schrödinger Software Suite</i> Dr. Sudharsan PANDIYAN, Principal Scientist, Schrödinger Inc.
16:20-17:00	Panel Discussion/ Closing Remarks