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DEPARTMENT OF ENERGY SCIENCE

[Energy Distinguished Lecture Series]

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AI for Advancing OLEDs: From Molecular Discovery to Device Physics

N Center #86120, Sungkyunkwan University, Suwon

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Abstract

Artificial intelligence (AI) is emerging as a powerful tool for bridging fundamental physics and practical materials engineering in organic light-emitting diodes (OLEDs). This talk introduces an AI-driven framework that spans from the design of new functional materials to the quantitative characterization of device physics.

The first part of the talk focuses on molecular discovery using generative AI. We design multi-resonance (MR) and donor-acceptor (D-A) type thermally activated delayed fluorescence (TADF) emitters and apply a high-throughput screening (HTS) process to efficiently filter a large library of AI-generated candidates and identify promising structures. The photophysical potential of the selected emitters is then validated by density functional theory (DFT) calculations.

The second part addresses the analysis of internal device dynamics. We have developed convolutional neural networks (CNNs) that interpret charge behaviors from operating voltages, as well as machine learning models that extract polaron recombination coefficients from transient electroluminescence (EL). In addition, we have established deep learning models that predict key kinetic parameters, including triplet-triplet annihilation (TTA) coefficients in blue OLEDs and reverse intersystem crossing (RISC) rates in TADF devices. These models address the uncertainties inherent in multivariable kinetic analysis and provide a quantitative understanding of exciton and polaron interactions. By combining generative molecular design with predictive device physics, this AI-driven approach offers an integrated pathway toward next-generation high-efficiency OLEDs.

Brief Bio



Jae-Min Kim received his B.S. and Ph.D. degrees from the Department of Materials Science and Engineering, Seoul National University, Korea, where he completed his doctoral research under the supervision of Prof. Jang-Joo Kim. He then joined Samsung Display as a staff engineer and worked on high-performance organic light-emitting diodes (OLEDs) for the Galaxy and iPhone series. He subsequently completed postdoctoral research in applied physics and artificial intelligence at Sungkyunkwan University.
He is currently an assistant professor in the Department of Advanced Materials Engineering at Chung-Ang University and a co-founder of EMITTING SQUARE Co., Ltd. His research interests include applied physics and modeling of organic photonic devices, as well as AI-assisted material and device design for OLEDs. His honors include selection among the 100 Outstanding National R&D Achievements of Korea, the UDC Innovative Research Award, the KIDS Award, and the Best Engineer Award from Samsung Display.

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