2026

PSK-이녹스 신진연구자 웨비나

2026년 2월 23일(월) AM 10:00 - 11:00 | 온라인 상
https://korea-ac-kr.zoom.us/j/2955276527

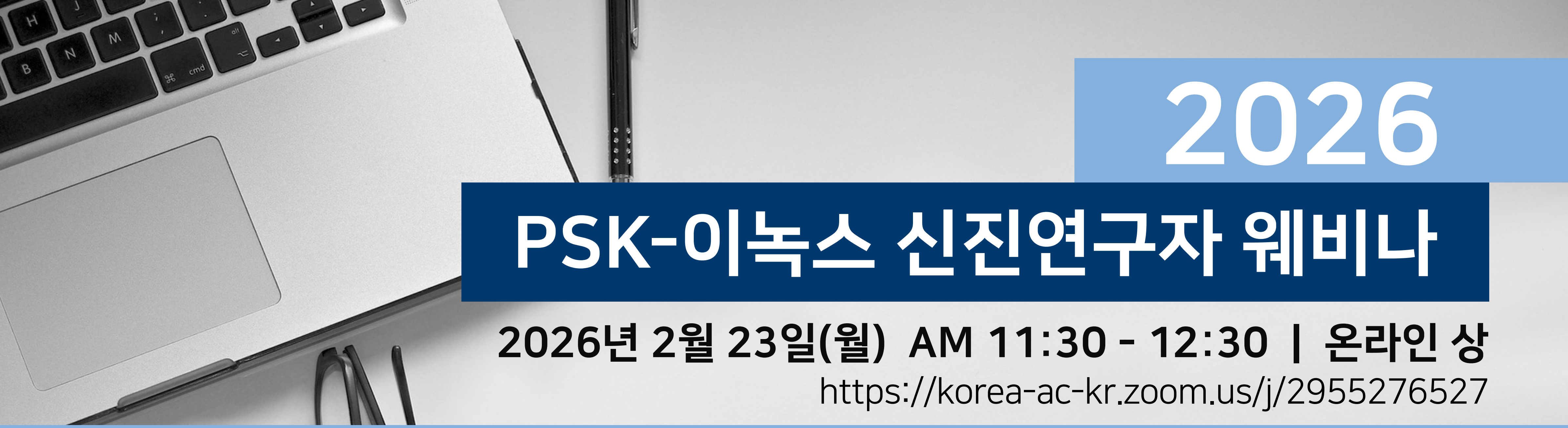
주최 한국고분자학회 **주관** 에너지 부문위원회 **후원** INNOX

○ 초대의 글

'PSK-이녹스 신진연구자 웨비나'는 우수한 연구역량을 가진 신진연구자를 발굴하여 교류의 장을 넓히고자 (주)이녹스의 후원과 한국고분자학회 주최로 마련한 온라인 세미나입니다. 이번 세미나에서는 고분자 분야 중에서도 특히 차세대 에너지 기술인 에너지 저장 분야에서 선도연구를 수행하는 신진연구자의 우수한 연구성과를 공유하는 자리를 마련하였으니 관심있는 분들의 많은 참여 부탁드립니다.

○ 일정

AM 10:00 - 11:00	Accelerating Electrocatalyst Discovery via Human–AI–Robot Collaboration Jiheon Kim (김지헌), jiheon.kim@utoronto.ca Postdoctoral Researcher, Department of Electrical and Computer Engineering & Department of Mechanical and Industrial Engineering, University of Toronto
	ABSTRACT: The integration of artificial intelligence (AI) with automated experimentation is rapidly reshaping the landscape of materials discovery. While substantial progress has been achieved in molecular discovery fields such as pharmaceuticals, optoelectronics, and photocatalysis, translating these advances to heterogeneous (electro)catalysis remains difficult. This challenge arises because the preparation of heterogeneous catalysts and the evaluation of their performance—especially under practically relevant electrolyzer conditions—are experimentally complex and difficult to scale with automation. Even when automation partially alleviates these constraints, efficiently navigating high dimensional optimization space still requires intelligent strategies for selecting and prioritizing experiments. This need has motivated the development of AI-driven autonomous laboratories aimed at accelerating experimental exploration. However, purely autonomous AI-driven strategies, despite their strengths in sparse-data regimes, often converge prematurely to local optima, limiting their ability to uncover truly high-performance materials. This talk presents an accelerated electrocatalyst discovery workflow that integrates robotic and high-throughput experimentation with interpretable AI models, enabling on-the-fly incorporation of domain expertise, allowing human insight to actively steer the discovery process. Particular focus is placed on accelerating the discovery of CO2 electrocatalysts for C3 hydrocarbon production, a reaction network of high intrinsic complexity that highlights the need for robust acceleration platforms capable of generating reliable and reproducible datasets. Using this framework, accelerated exploration of practical catalyst compositions and the extraction of data-driven mechanistic insights that inform the design of complex electrocatalytic systems are demonstrated. The talk concludes by discussing future directions for the field, highlighting pathways toward more scalable and reliable AI-driven experimental discovery.



2026

PSK-이녹스 신진연구자 웨비나

2026년 2월 23일(월) AM 11:30 - 12:30 | 온라인 상

https://korea-ac-kr.zoom.us/j/2955276527

주최 한국고분자학회 **주관** 에너지 부문위원회 **후원** INNOX

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○ 일정

AM 11:30 - 12:30	From Coordination Environment to Reactivity: Orbital Tuning in Single Atom Electrocatalysts Kiwon Kim (김기원), kiwon.kim.2016@gmail.com Postdoctoral Researcher, Department of Chemical Engineering, Cornell University

ABSTRACT: Electrocatalytic reactions for electrochemical water splitting are governed by the electronic structure of active sites, particularly the interaction between the d or p orbital of active sites and reaction intermediates. In this talk, I present a ligand engineering strategy for single atom electrocatalysts, demonstrating how precise control of local coordination environments modulates orbital occupancy, spin state, and adsorption energetics. By tailoring the local coordination environment surrounding isolated transition metal atoms, the electronic structure of the metal center can be systematically modulated, including crystal field splitting, orbital occupancy, and spin state. These changes directly influence adsorption strength and reaction kinetics, enabling control over activity and stability across key electrochemical reactions. Combined operando spectroscopic measurements and theoretical calculations reveal that subtle variations in metal–ligand geometry can shift orbital alignment and antibonding interactions, creating electronically optimized active sites under both acidic and alkaline conditions. This work highlights how ligand controlled orbital tuning provides a unifying strategy to bridge molecular level concepts with robust heterogeneous electrocatalysts for energy conversion.

한국고분자학회
The Polymer Society of Korea