NUS National University of Singapore | Department of Materials Science & Engineering
College of Design and Engineering

Department Seminar

Dear Colleagues & Students,
You are cordially invited to a special seminar on

Date: 7 July 2026, Tuesday
Time: 4pm
Venue: E4-04-05 E-Cube 1, 4 Engineering Drive 3, #04-05, Singapore 117583 (Map)

Atomically precise layer-by-layer titration of perovskite oxides reveals the termination-specific reactivity in oxygen electrocatalysis

By Dr. Di Chen
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Hosted by Dr. Xianwen Mao

Abstract:
Advances in *in situ* characterization have enabled increasingly detailed studies of surfaces and interfaces.[1] The oxygen incorporation reaction (OIR) is a key process in solid-state electrochemistry and underpins technologies such as solid oxide fuel cells, thermochemical water and carbon dioxide splitting, oxygen-transport membranes, and environmental catalysis.[2] However, how atomic-scale surface structures regulate OIR remains poorly understood. A longstanding debate concerns the role of SrO on perovskite cathodes: it is often considered detrimental, yet recent studies suggest that it may enhance surface kinetics. To resolve this controversy, we developed an in situ atomic-layer titration platform for layer-by-layer control and activity measurement of $(La_{0.5}Sr_{0.5})FeO_3$−δ thin-film surfaces.[3] We observed a volcano-shaped dependence of OIR activity on SrO coverage, with a single SrO layer delivering an activity approximately 30 times higher than that of the FeO_2-terminated surface. Microkinetic modelling and first-principles calculations showed that surface termination changes the rate-determining step from molecular oxygen dissociation to atomic oxygen incorporation or diffusion. The single SrO layer provides an optimal balance among oxygen dissociation, incorporation, and subsurface transport. These results establish a quantitative link between catalytic activity and surface atomic structure, offering an atomic-scale strategy for designing oxide electrocatalysts.

Ref:

[1] Xianwen Mao, Di Chen, T. A. Hatton* et al., Nature Materials **18**, 1350–1357 (2019).*
[2] Di Chen, William C. Chueh et al., Nature Catalysis **3**, 94–105 (2020).*
[3] Hongyang Su, Di Chen et al., Nature Catalysis, online, (2026).*

Biography:
Di Chen is an Associate Professor in the Department of Building Environment and Energy Engineering at The Hong Kong Polytechnic University, with a joint appointment in the Department of Chemistry. He received his B.S. from Tsinghua University, Ph.D. from MIT, and postdoctoral training at Stanford University, all in Materials Science and Engineering. Before joining PolyU in July 2026, he was an Associate Professor （副研究员） and later Professor （研究员） in the research track at Tsinghua University's Future Laboratory. His research focuses on surface electrocatalysis and its applications in energy and environmental technologies, including solid oxide fuel cells, automotive exhaust catalysis, and antimicrobial architectural ceramics. He has led projects including the National Key R&D Program of China, the National Natural Science Foundation of China, and industry partners.