UC Irvine Samueli
Department of Chemical and Biomolecular Engineering

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11:00 am – 12:00 pm

Synergistic Effects in Oxygen Evolution catalysis – in-situ X-ray based approaches

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Abstract: Electrolytic hydrogen production is one of the defining technologies supporting the large-scale deployment of renewable energy sources. Although the water electrolysis integrates two complementary processes – 2 electron hydrogen evolution (HER) and 4 electron oxygen evolution (OER)most of the development efforts concentrates on OER which is known to be energy demanding and often limiting the overall electrolysis efficiency. Current understanding of OER based on DFT modelling [1] identifies intrinsic kinetic constraints of the process resulting from so called scaling relations. The restrictions of the scaling relations are summarized in the theoretically constructed volcano plot which predicts noble metal based oxides like, e.g. ruthenium oxides (RuO_2) and iridium oxides (IrO_2) to be the best OER catalysts. The restrictions of the theoretically predicted volcano were apparently removed for several binary oxide system exploring coexistence Ru-Ni [2], Ru-Ir [3] in the structure which shows synergistic improvement of OER activity. A similar activity improvement in activity has been observed in alkaline media for Ni-Fe-based catalysts. This type of behavior arises from co-existence of cations residing on opposite sides of the so-called “oxo-wall”. The lecture will present combined theoretical and experimental rationalization of this synergistic behavior stressing the role of the spectator site activation in removing the scaling relations restrictions. The theoretical predictions for OER catalysts in Ru-Ir system and Ni-Fe binary systems will be compared with results of in-situ and operando soft X-ray absorption spectroscopy (XAS) and operando X-ray photoelectron spectroscopy (XPS).

Bio: Petr Krtil is an alumni of the University of Chemistry and Technology in Prague. He received a PhD in Physical Chemistry from the J. Heyrovsky Institute of Physical in Prague in 1993. Following two postdoctoral appointment at State University of New York at Buffalo (S. Bruckenstein, 1994) and at Tokyo Institute of Technology (M. Yoshimura, 1997) he re-joined the J. Heyrovsky Institute of Physical Chemistry as a senior scientist. In addition to his research appointment at the J. Heyrovsky Institute he has been appointed an Associate Professor of Physical Chemistry at the Technical University Dresden (2012-2022). He was appointed a professor of Inorganic Technology at the University of Chemistry and Technology in Prague in 2023. He also keeps teaching appointment at the Faculty of Mathematics and Physics of the Charles University in Prague. His research focused on development of complex materials for electrochemical energy conversion and storage. His most recent interests concentrate on *in situ* and *operando* characterisation of catalytic systems, particularly through advanced soft X–ray–based techniques.

References: [1] I.C. Man, H.-Y. Su, F. Calle-Vallejo, H.A. Hansen, J.I. Martínez, N.G. Inoglu, J. Kitchin, T.F. Jaramillo, J.K. Nørskov, J. Rossmeisl, Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces, ChemCatChem, 3 (2011) 1159-1165.

[2] R.K. Pittkowski, D.F. Abbott, R. Nebel, S. Divanis, E. Fabbri, I.E. Castelli, T.J. Schmidt, J. Rossmeisl, P. Krtil, Synergistic effects in oxygen evolution activity of mixed iridium-ruthenium pyrochlores, Electrochimica Acta, 366 (2021) 137327.

[3] Lalita Sharma, Roman Nebel, Katrine Svane, Kaoruho Sakata, Kateřina Minhová Macounová, Rebecca K. Pittkowski, Henrik H. Kristoffersen, Mariana Klementová, Kenta Amemiya, Jan Rossmeisl, and Petr Krtil, Synergetic Effects in Oxygen Evolution on Ru-Ir-O Solid Solutions: A DFT and In-Situ Soft X-ray Absorption Spectroscopy Study, ACS Catalysis, 2026, 16, 9, 8008-8021.

Hosted by: *Prof. Iryna Zenyuk*