서울대학교 에너지 이니셔티브 연구단

초청세미나

Unified quantum theory of electrochemical kinetics By coupled ion-electron transfer

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- 일시 : **2025/8/27, 5:00pm-6:00pm**
  301동 102호 (Building no.301, room 102)

◆ Abstract

The Butler-Volmer (BV) equation, originally developed to fit Tafel's rate law for electrolysis, has become the standard model for electrochemical reaction kinetics, and yet a century later, it still lacks a clear microscopic basis. In 1936, Butler derived the BV equation from Gurney's seminal "quantum theory of electrolysis" (1932), which assumes electron transfer (ET) of "neutalization" is a fast step coupled to classical proton transfer. In 1956, Marcus famously challenged this picture with his theory of ET coupled to solvent reorganization, rather than ion transfer. Here, we present a unified quantum theory of coupled ion-electron transfer (CIET), which leads to a simple rate formula that smoothly interpolates between Marcus-like and BV-like kinetics, depending on whether electron- or ion-transfer is rate limiting, respectively.[1] CIET theory provides a powerful link between quantum chemistry and electrochemical engineering, as illustrated by examples of ET-limited reaction kinetics in Li-ion[2] and Li-air[3] batteries and IT-limited reaction kinetics in electrocatalysis. For the first time, the theory predicts the metal-work-function dependence of BV kinetics for the hydrogen evolution reaction (HER) in acid and provides a mathematical framework to predict electrochemical reaction rates from ab initio quantum simulations, as recently demonstrated for lithium cobalt oxide (LCO) batteries with different electrolytes.[4]

◆ Biography

Martin Z. Bazant is the E. G. Roos (1944) Professor of Chemical Engineering and Mathematics at the Massachusetts Institute of Technology and a member of the National Academy of Engineering. After a Ph.D. in Physics at Harvard (1997), he joined the MIT faculty in Mathematics (1998) and then Chemical Engineering (2008), where he served as Executive Officer of the Departement from 2016 to 2020. His awards include the Kuznetsov Prize in Theoretical Electrochemistry (ISE), the Acrivos Award in Chemical Engineering (AIChE), and the MITx Prize for Teaching in MOOCs. He is a fellow of the International Society of Electrochemistry, the Electrochemical Society, the Royal Society of Chemistry, and the American Physical Society. He serves as President of the International Electrokinetics Society, Director of the D3BATT Center for Data-Driven Design of Batteries (Toyota Research Institute), Director of the Center for Battery Sustainability (MIT-Northeastern), and Chief Scientific Advisor for Saint-Gobain Research North America. He is also the Chief Scientist and Co-founder of Lithios, Inc. commercializing Advanced Lithium Extraction (ALE) from brines.

Host : 전기정보공학부 김성재 교수 (gates@snu.ac.kr)

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