Beyond Linear Scaling: Innovations in Catalyst Optimization

Kihyun Shin[1]*, Hyun You Kim[2], Kyubock Lee[3]

[1]Department of Materials Science and Engineering, Hanbat National University, Daejeon 34158, Republic of Korea

[2]Department of Materials Science and Engineering, Chungnam National University, Daejeon 34134, Republic of Korea

[3]Graduate School of Energy Science and Technology, Chungnam National University, Daejeon 34134, Republic of Korea

Recent studies in electrochemical reaction simulations have revealed the construction of Volcano plots and 2D contour plots based on a strong linear scaling relation between the adsorption energies of intermediate species. This linear scaling relation provides researchers with a straightforward descriptor to predict catalyst performance and enables the visualization of large datasets of catalyst performance on simple contour plots. However, to maximize catalyst performance, it is crucial to identify outliers that do not follow the linear scaling relation. Particularly in the oxygen reduction reaction (ORR), a strong linear scaling relation between OH and OOH adsorption energies sets clear limits on catalyst activity. Overcoming these limits requires understanding how outliers arise and how researchers can control them. In this presentation, we will explore the fundamental assumptions and theories of electrochemical catalyst simulations and examine how Volcano plots and 2D contour plots are formed based on the linear scaling relation. Additionally, we will investigate the impact of ensemble, electronic, and strain effects on adsorption energies and explore various possibilities for generating outliers that deviate from the linear scaling relation.