CONCEPT PAPER

for KIER International Cooperation project

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Title	**Model electrode study for electrochemical devices by combining theoretical and experimental insights**			
Description	__ Barrier to tackle: Electrochemical devices are of interest for uses for energy conversion and storage application since it possess a lot of advantages, such as low cost, long life span, high energy-power density, good reversibility, and pollution-free operation. At present, however, the sluggish kinetics of electrode reaction still limit the efficiency of fuel cells, supercapacitor, and secondary ion battery, *i.e.*, the oxygen reduction/evolution reactions for fuel cell and charge transfer reactions for both supercapacitor and secondary ion battery. Despite the important role of electrode reaction kinetics on the viability of these devices, the governing mechanisms remain elusive and poorly understood. The proposed work is primarily aimed at understanding the kinetics of surface oxygen exchange on the model electrodes (Pt/C, carbon-based materials, oxide-based materials, etc.), and its relationship with surface morphology and bulk structure. __ Strategy to solve: A unique combination of advanced techniques, comprising ^{18}O-^{16}O pulse isotopic exchange, electrochemical impedance spectroscopy, and electrical conductivity relaxation will be used to study the electrode reaction kinetics. Several studies on different materials will be conducted to explore the elementary steps involved in the oxygen reduction/evolution reactions and charge transfer reactions, and to determine the role of surface composition, microstructure and bulk chemistry. Low energy ion scattering, together with transmission electron microscopic analyse, will be employed for characterisation of the surface microstructure and elemental composition. First principles atomistic calculations will performed to address how surface chemistry accelerates the electrode reaction process.			
Outcomes*	__ Detailed experimental evaluation of electrode reaction kinetics of at least three material systems (single phase and/or composites). __ Mechanistic and atomistic scale modeling of the detailed electrode reactions. __ 4 Publications in peer reviewed journals and/or patents.			