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Atomic-level perspective on the functionality of nanoalloy catalysts inside operating fuel cells by combined in operando high energy X-ray spectroscopy and total scattering

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The activity and stability of nanoalloy catalysts for the chemical reactions driving devices for clean energy conversion, such as the oxygen reduction reaction (ORR), depend critically on optimizing the composition, surface area and phase type of the nanoalloys, including the bonding interactions between the constituent atoms, for the harsh operating conditions inside the devices. We present results from in operando high-energy X-ray diffraction (HE-XRD) study coupled by atomic pair distribution function (PDF) analysis and energy dispersive X-ray spectroscopy (EDS) on the concurrent atomic-scale changes and decay of the ORR activity of Pd-Sn, Pt-Ni-Cu nanoalloy catalysts as they function at the cathode of a proton exchange membrane fuel cell (PEMFC). Here, we address the problem by studying the atomic-level evolution of noble metal-based nanoalloy catalysts for ORR as they function at the cathode of an actual proton exchange membrane fuel cell (PEMFC). We use 1-min time and μm -sized space resolved energy dispersive X-ray spectroscopy (EDS) and total X-ray scattering to obtain precise information about the chemical composition, geometric surface area, phase content, 3D arrangement and strength of interaction between the constituent atoms of the nanoalloys. Besides, we evaluate the utilization of the nanoalloy catalysts by measuring variations in their chemical composition and mass distribution over the PEMFC cathode. Concurrently, we measure the current output of the cell that reflects the ORR activity of the nanoalloys. Experimental X-ray data show that the atomic-level changes of nanoalloys can occur simultaneously over different time frames, ranging from minutes-long structural phase transitions to hours-long alterations in chemical composition, and in multiple dimensions, ranging from repetitive sub-Å atomic displacements to nm-sized particle growth. Besides, X-ray data reveal considerable exchange of atomic species between individual nanoalloy particles, that is, effective mass transport across the PEMFC cathode. Experimental catalytic data show that the ORR activity of nanoalloys closely tracks the atomic-level changes they undergo during the PEMFC operation. Ultimately, we demonstrate the great potential of combined in operando EDS and PDF studies as a tool for guiding the effort to produce more efficient and affordable nanocatalysts for energy related applications.

Biography

Yazan Maswadeh is an experienced Research Assistant working in Material Science field. He is skilled in HE-XRD, EDS, XPS, data analysis and data mining. The latest project in which he works on is about the structural dynamics and activity of nanocatalysts inside fuel cells by high energy X-ray diffraction (HE-XRD) coupled with in-operando atomic pair distribution studies (PDF), cyclic voltammetry (CV), x-ray energy dispersive spectroscopy (EDX) and molecular dynamics (MD). To reveal the activity and stability of nanoalloy catalysts for chemical reactions driving devices for clean energy conversion.

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