International Institute for Carbon-Neutral Energy Research

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Electrochemical Energy Conversion Roadmap Revision

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Division Objective

This division conducts fundamental studies on the two essential components for the electrochemical energy conversion, that is electrodes and electrolytes,

- To understand and tailor the chemistry of surfaces, interfaces and the intrinsic nature of electrodes,
- To comprehend, control, and design ion conduction in electrolytes.

Technological development for energy-efficient and robust electrochemical energy conversion is perused as outcomes of the fundamental electrode and electrolyte studies for the following devices:

- Polymer electrolyte cells
- Solid oxide cells
- Energy storage

Division Projects, Objectives, Research Efforts

Projects	Objective	Research Efforts	Researchers
Project 1 Electrodes	**Understanding and tailoring the chemistry of surfaces, interfaces and the intrinsic nature of electrode materials.** • Elucidating fundamental processes in electrochemical reactions and electrode degradation phenomena. • Use of these insights to design novel, more efficient, durable electrode materials for polymer electrolyte cells (PECs) and solid oxide cells (SOCs).	• Electrochemical analysis and design for platinum electrocatalysts in PECs. • Investigation of Pt-free Fe/N/C electrocatalysts for PECs. • Design of functional carbons for enhanced use in PEC electrodes. • Advanced metal-oxide electrode characterization and design assisted by surface analysis • Understanding and tailoring of chemical expansion in solid electrodes • Protonic mixed-conducting electrodes	Nakashima, Fujigaya, Gewirth Sasaki, Lyth, Hayashi, Kilner, Tellez, Druce, Tuller Perry, Bishop, Matsumoto
Project 2 Electrolytes	**Comprehension, control, and design of ionic conduction** • Highly durable polymer electrolytes with high conductivity and low crossover at low humidity and in wide temperature range. • Understanding electro-chemo-mechanical effects in metal oxides for enhanced ion conductivity and stability. • Study of proton-conduction in metal oxides for low-temperature solid electrolytes	• High temperature, low humidity polymer electrolytes for PECs. • Novel low dimensional ionomers for PECs: nanoparticles, nanofibers and nanosheet membranes • Electro-chemo-mechanics for ionic and mixed conductors • Fundamental understanding of proton conduction in metal oxides to develop high proton conductors	Fujigaya, Sasaki, Lyth, Nishihara, Kilner, Tellez, Druce, Tuller, Perry, Bishop, Matsumoto, Ertekin, Staykov

Division Projects, Objectives, Research Efforts

Projects	Objective	Research Efforts	Researchers
Project 3-1 Polymer electrolyte cells	**Fabrication and characterization of advanced PEFCs and PEECs** • high durability, high efficiency • Wide temperature range • Low Pt loading / Pt-free	• Highly durable PEFCs based on advanced polymer-coated carbon electrocatalyst • Operation of Pt-based / Pt-free HT-PEFCs • Development of new cell architectures for water electrolysis using low-dimensional ionomer membranes • Novel device and system design for PEECs.	Nakashima, Fujigaya, Lyth Matsumoto, Ito
Project 3-2 Solid oxide cells	**Advanced SOFC** • Based on newly tailored electrodes and electrolytes • Ultra high efficiency hydrogen-fueled SOFC **Electrolysis of water and other chemical species** • Thermally self-standing and endothermic operation of steam electrolysis • Material design and durability for oxidative and reducing environment	• Nano-structured electrodes for reduced-temperature operation of SOFC/SOEC • Next generation SOFC/SOEC utilizing the tailored electrodes and electrolytes for extreme efficiency operating at reduced temperatures • Hydrogen-fueled SOFC • Proton-conductor-based SOEC • Oxide-ion-conductor-based SOEC	Matsumoto, Tuller Perry, Bishop, Kilner Druce, Tellez, Rupp, Ishihara
Project 3-3 Energy storage	• High capacity new concept batteries • PEFC/PEEC and SOFC/SOEC • Sufficient round-trip efficiency	• Dual carbon battery • Fe-air battery • SOFC/SOEC reversible cells and systems • PEFC/PEEC reversible cells and systems	Ishihara, Kilner, Druce, Tellez, Matsumoto, Nakashima, Gewirth Fujigaya, Ito

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Milestones

	2014-2020 (short)	2021-2025 (mid)	2025-2030 (long)
Project 1 Electrodes	PEC: Theory of minimizing overpotential up to 120°C	PEC: Combine durability with improved activity: mass activity >0.4 W/mg_{Pt} up to 150°C	Operation at ~180°C, low mas activity (>0.45 W/mg_{Pt}), negligible degradation over 10^5 potential cycles with deep theoretical grasp
	PEC: Durable electrodes through novel design: 10^5 potential cycles	PEC: Elucidation of reaction kinetics at high temperature	Chemically engineered no-Nafion carbon-based electrodes for PECs
	Pt-free electrode: Elucidation of roles of C, N, Fe in active site	Pt-free electrode: Negligible degradation, improved efficiency (<5% H_2O_2)	
	Establishment of quantification of surface chemistry by LEIS/SIMS		
	SOC: Highly active stable electrode : $D^*k=10^{-17}$ $cm^3\ s^{-2}$ at 500°C	SOC: Understanding of surface exchange degradation mechanisms	Tailored metal-oxide electrode demonstrating long-term stable, rapid surface exchange and reduced chemical expansion
	Factors impacting chemical expansion in perovskites identified and understood	Quantitative and predictive theory of oxygen exchange in terms of composition and defect chemistry	
	Protonic air electrode $\eta<0.15$ V@0.5 A/cm^2, 500°C	Protonic air electrode $\eta<0.15$ V @0.5 A/cm^2, 500°C	Protonic anode and cathode with $\eta<0.15$ V@0.5 A/cm^2, below 300°C
Project 2 Electrolytes	New polymer electrolytes: 10^{-2} S/cm at 0-120°C (RH=30%)	New polymer electrolytes: 10^{-2} S/cm at 0-150°C (RH=30-90%)	New polymer electrolytes: 0.1 S/cm at 0-180°C (RH=10-90%)
	Fundamentals of nanoconfined and surface proton conductivity mechanism in nanomaterials.	Novel ionomer: 10^{-2} S/cm at 120°C, H2 permeability <0.1 barrer, durability ~1000 h	Thin (<100 nm), low cost, printed electrolyte membranes with 10^{-1} S/cm at 180°C, H_2 permeability<10^{-3} barrer, durability>10000 h
	Factors impacting chemical expansion of proton conductors identified	Strain-induced high ion-conducting solid oxides (e.g. 10^{-1} S/cm at 500°C), grain boundary chemistry understood for fast transport	Ion-conduction enhancement by strain and/or space-charge in solid electrolytes
	New protonic solid oxide electrolytes: 10^{-2} S/cm at 500°C	New protonic solid oxide electrolytes: 10^{-2} S/cm at 500°C	New protonic solid electrolytes: 10^{-2} S/cm below 300°C

Milestones

	2014-2020 (short)	2021-2025 (mid)	2025-2030 (long)
Project 3-1 Polymer electrolyte cells	Highly durable electrode by polymer-coating with Pt loading<0.5 g/kW Pt-based PEFC operation at 150°C Pt-free PEFC at 90°C, 0.15 W/cm^2 Novel PEC: Electrode-supported membranes (5 μm, OCV>0.90 V) Water electrolysis: High efficiency >80% (HHV)	PEFC: Pt loading <0.1 g/kW High durability at 150°C using new materials for Pt- and Pt-free PEFCs Novel PEC: Membrane deposition by printing to operate at elevated temperature (120°C, OCV > 0.97 V) Water electrolysis: Thermally-self-standing operation at RT-120°C.	Pt-free & low-Pt PEFCs operating up to 180°C with high durability, power density and efficiency PECs with thin-film nanomaterial membranes, high OCV (> 1 V) and high energy Pressurized, highly stable water electrolysis at 1.4 V.
Project 3-2 Solid oxide cells	Fabrication and testing of cells with nanostructured electrodes Illustration of SOFC based on new electrodes and electrolytes H_2-fuel SOFC 0.5 W/cm^2 at 500°C SOEC 90% HHV efficiency at 500°C, 0.5 A/cm^2	Understanding of durability nanostructured electrode SOFC involving strain/space-charge effect H_2-fuel SOFC 0.5 W/cm^2 at 400°C SOEC: Thermal self standing operation 0.5 A/cm^2 and 90% HHV efficiency at 2.0 A/cm^2, at 500°C	Nano-structured electrode η<0.2 V at 0.5A/cm^2, 500°C H_2-fuel SOFC 0.5 W/cm^2 below 400°C (for portable use) SOEC: operation at 500°C with degradation < 0.5%/ 1000 h
Project 3-3 Energy storage	Novel battery: Proposal of new concept Establishment of electrodes for dual mode operation for PEC Reversible PEFC/PEEC operation at 120-150°C, roundtrip efficiency~50% Reversible SOFC/SOEC: roundtrip efficiency~60%	Novel battery: Efficiency>90%, Capacity 200Wh/kg Reversible PEFC/PEEC operation at 120-150°C, roundtrip efficiency>60% Reversible SOFC/SOEC: roundtrip efficiency>70%	

Ultimate Targets

	Ultimate targets	Current Benchmarks
Project 1 Electrode	For PECs • Stable half-cell operation for 100,000 potential cycles • Pt-free electrocatalyst with high activity 0.44 A/g at low cost For SOCs • Stable and durable solid oxide electrode material with D*k>10^{-14} cm^3 s^{-2} at 500°C, with acceptable stability • Chemical expansion coefficient<0.01 • Comprehensive atomistic understanding of electrode processes in relevant materials	ECSA degradation below 10% under FCCJ condiciton after 10,000 cycles.. Pajareto Powder: 0.17 A/g, 200 $/g D*k = 10^{-19} cm^3 s^{-2} (LSCF, 500°C) Little theoretical work on technologically relevant materials
Project 2 Electrolyte	Polymer electrolytes • Conductivity comparable to Nafion (>0.05 S/cm) • Low cost (<40 USD/m^2) • Stable operation at 180°C for 10,000 hours. Solid oxide electrolytes • Cross-plane ionic conductivity>0.01 S/cm at 300°C (protons) or 500°C (oxide ions) with ionic transport number>0.99	Nafion: 0.1 S/cm Nafion: 1400 USD/m^2 Nafion: 90°C; PBI: 180°C 0.05 S/cm at 500°C ($Bi_2V_{1.9}Cu_{0.1}O_{5.35}$) 0.016 S/cm at 500°C (GDC) 0.006 S/cm at 500°C (LSGM)

Ultimate Targets

	Ultimate targets	Current Benchmarks
Project 3-1 Polymer electrolyte cell	PEFC • Operation temperature: 0-180°C • Electrode: low Pt-loading (< 0.1 mg/cm^2) or Pt-free • Non-humidifying operation Water electrolysis • Cell voltage: 1.5 V@1 A cm^{-2} (thermo-neutral), 1.6 V@2 A cm^{-2}	Nafion: 0-90°C, PBI: 80-180°C, 0.7 g/kW non-humidifiying operation below 80°C Cell voltage: 1.7 V@2 A/cm^2, J. Xu et al., 2012
Project 3-2 Solid oxide cell	• Operation temperature: 300-500°C • Durability:0.5%@1000hrs. • SOEC: > 1 A cm^{-2} under thermo-neutral operation (~1.3 V) • SOFC: 1-5 W/cm^2	SOEC: 1 A cm^{-2} (@800°C) with 2% / 1000h degradation – Sun et al. (DTU, Denmark)
Project 3-3 Energy storage	New battery: • Overall Energy Efficiency >90%, • Capacity; 300 Wh/kg • Rate Property; 70% discharge capacity @ 10C FC-EC reversible energy storage • SOFC/SOEC roundtrip efficiency >70% at 500°C • PEFC/PEEC roundtrip efficiency >60% • Degradation less than 0.5%/1000 h under reversible operation at 500°C with electrolysis current 1 A cm^{-2} at thermo-neutral voltage (1.3 V)	88% (Li ion battery) Capacity 200 Wh/kg Rate Property, 50% @5C Roundtrip efficiency >70% at 680°C (SOC) Roundtrip efficiency 42% (PEC) 4000h reversible operation at 800°C; 1 A/cm^2 @ 1.33 V in SOEC mode, 0.5 A/cm^2 in SOFC mode for 4000h