International Institute for Carbon-Neutral Energy Research

Electrochemical Energy Conversion Roadmap Revision

Revised, May 24, 2017

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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**

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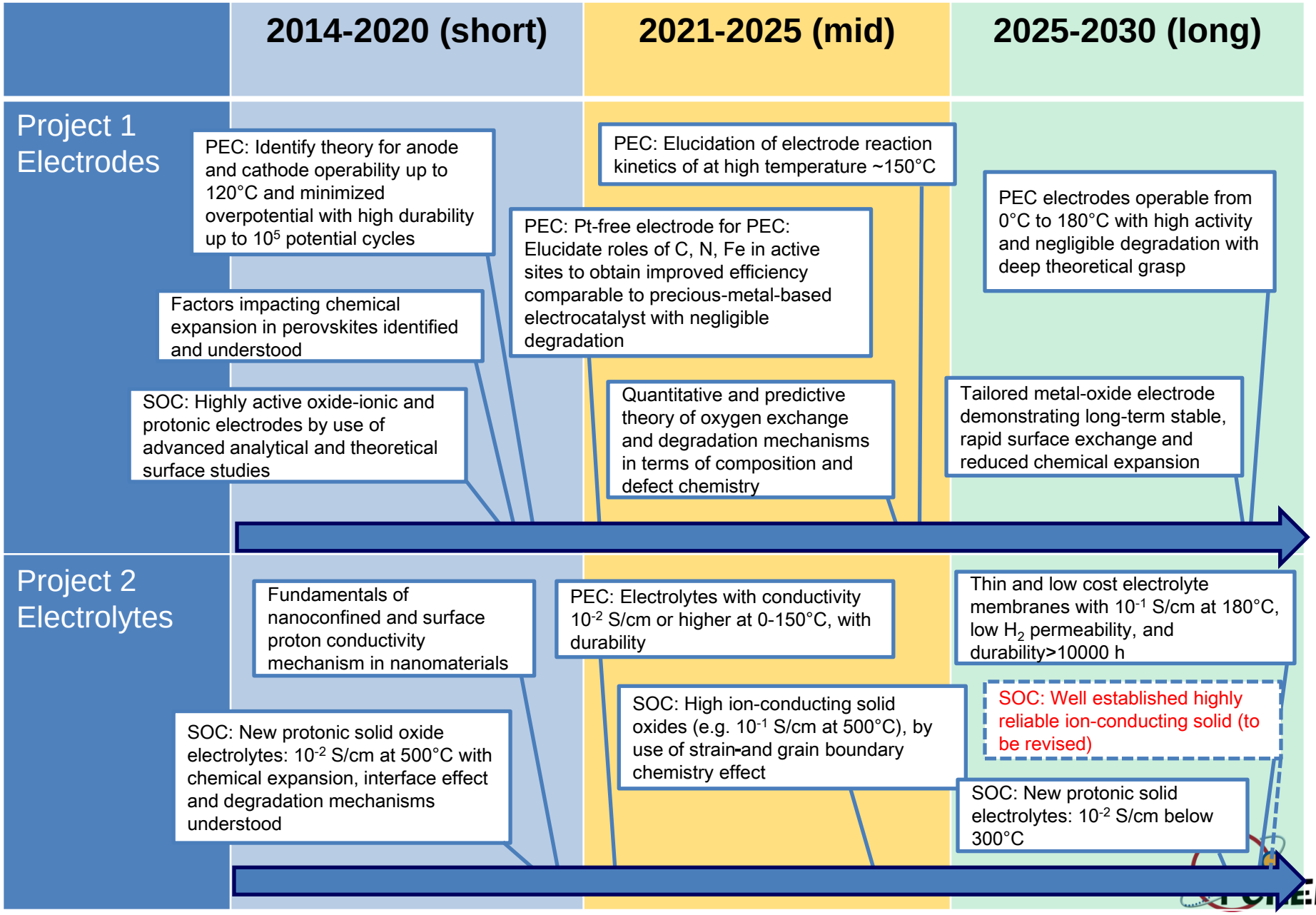
Division Projects, Objectives, Research Efforts

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).	• Investigation of Pt-free Fe/N/C electrocatalysts for PECs. • Design of functional materials and layered structure for enhanced use in PEC electrodes. • Advanced metal-oxide electrode characterization and design assisted by surface analysis and computation • Understanding and tailoring of chemical expansion in solid electrodes • Protonic mixed-conducting electrodes	Nakashima, Fujigaya, Gewirth Sasaki, Lyth, Kilner, Tellez, Druce, Tuller Perry, Matsumoto, Thoreton, Ghuman, Wu
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 conductivity proton conductors	Fujigaya, Sasaki, Lyth, Nishihara, Kilner, Tellez, Druce, Tuller, Perry, Bishop, Matsumoto, Ertekin, Staykov, Thoreton, Ghuman, Wu

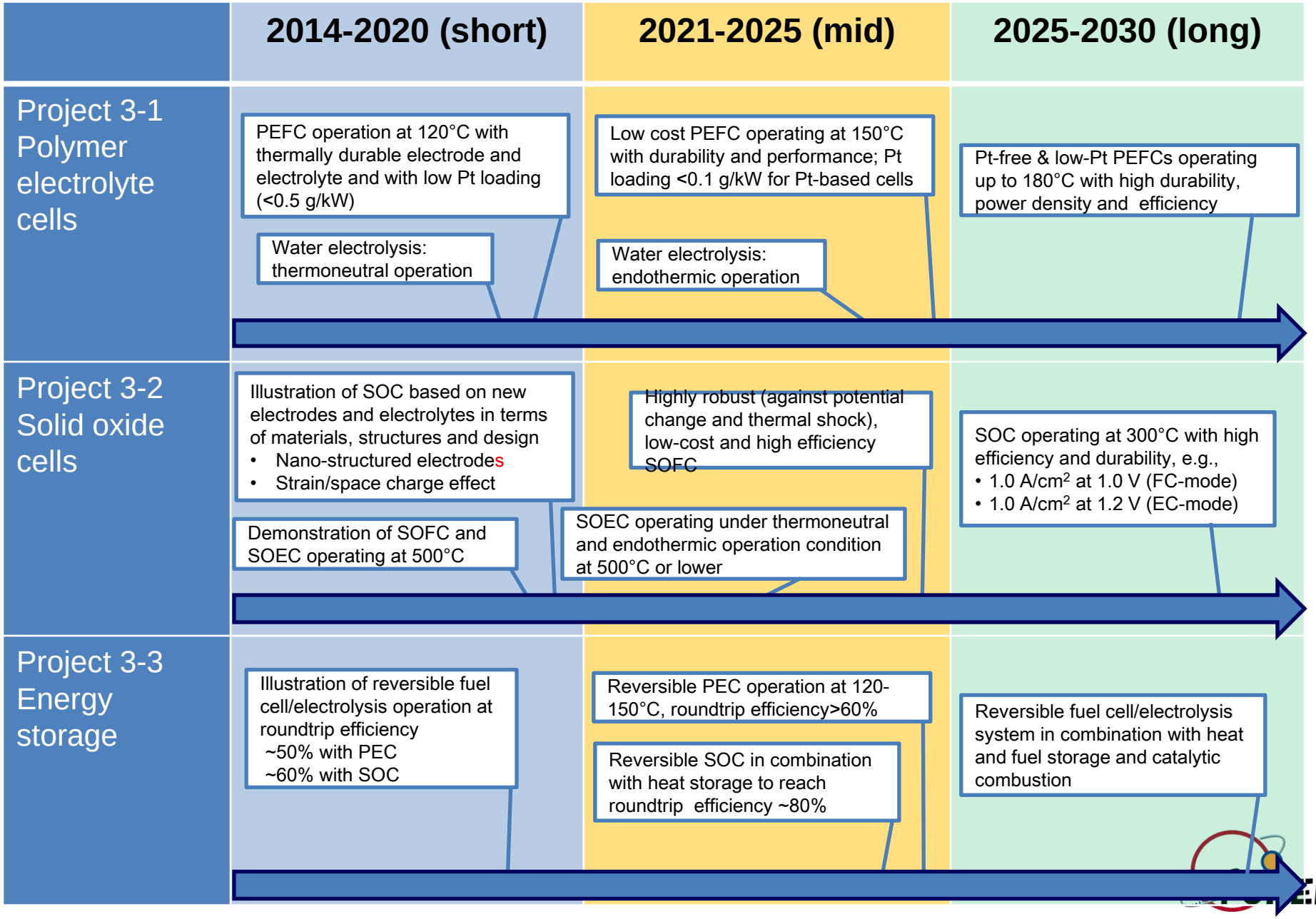
Division Projects, Objectives, Research Efforts

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 and PEECs 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	Nakashima, Fujigaya, Lyth Matsumoto, Ito, Ghuman
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	• 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, Kilner Druce, Tellez, 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

Milestones


2014-2020 (short)
2021-2025 (mid)
2025-2030 (long)
Project 1 Electrodes
PEC: Identify theory for anode and cathode operability up to 120°C and minimized overpotential with high durability up to 10^5 potential cycles
PEC: Elucidation of electrode reaction kinetics of at high temperature ~150°C
PEC: Pt-free electrode for PEC: Elucidate roles of C, N, Fe in active sites to obtain improved efficiency comparable to precious-metal-based electrocatalyst with negligible degradation
PEC electrodes operable from 0°C to 180°C with high activity and negligible degradation with deep theoretical grasp
Factors impacting chemical expansion in perovskites identified and understood
SOC: Highly active oxide-ionic and protonic electrodes by use of advanced analytical and theoretical surface studies
Quantitative and predictive theory of oxygen exchange and degradation mechanisms in terms of composition and defect chemistry
Tailored metal-oxide electrode demonstrating long-term stable, rapid surface exchange and reduced chemical expansion
Project 2 Electrolytes
Fundamentals of nanoconfined and surface proton conductivity mechanism in nanomaterials
PEC: Electrolytes with conductivity 10^-2 S/cm or higher at 0-150°C, with durability
Thin and low cost electrolyte membranes with 10^-1 S/cm at 180°C, low H2 permeability, and durability>10000 h
SOC: New protonic solid oxide electrolytes: 10^-2 S/cm at 500°C with chemical expansion, interface effect and degradation mechanisms understood
SOC: High ion-conducting solid oxides (e.g. 10^-1 S/cm at 500°C), by use of strain-and grain boundary chemistry effect
SOC: Well established highly reliable ion-conducting solid (to be revised)
SOC: 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
PEFC operation at 120°C with thermally durable electrode and electrolyte and with low Pt loading (<0.5 g/kW)
Water electrolysis: thermoneutral operation
Low cost PEFC operating at 150°C with durability and performance; Pt loading <0.1 g/kW for Pt-based cells
Water electrolysis: endothermic operation
Pt-free & low-Pt PEFCs operating up to 180°C with high durability, power density and efficiency
Project 3-2 Solid oxide cells
Illustration of SOC based on new electrodes and electrolytes in terms of materials, structures and design
• Nano-structured electrodes
• Strain/space charge effect
Demonstration of SOFC and SOEC operating at 500°C
Highly robust (against potential change and thermal shock), low-cost and high efficiency SOFC
SOEC operating under thermoneutral and endothermic operation condition at 500°C or lower
SOC operating at 300°C with high efficiency and durability, e.g.,
• 1.0 A/cm2 at 1.0 V (FC-mode)
• 1.0 A/cm2 at 1.2 V (EC-mode)
Project 3-3 Energy storage
Illustration of reversible fuel cell/electrolysis operation at roundtrip efficiency
~50% with PEC
~60% with SOC
Reversible PEC operation at 120-150°C, roundtrip efficiency>60%
Reversible SOC in combination with heat storage to reach roundtrip efficiency ~80%
Reversible fuel cell/electrolysis system in combination with heat and fuel storage and catalytic combustion

Ultimate Targets

	Ultimate targets	Current Benchmarks
Project 1 Electrode	For PECs • Stable ~~cell operation~~ electrode for 100,000 potential cycles in temperature range 0-180°C • Pt-free electrocatalyst having comparable catalytic activity to precious-metal-based catalyst 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 solid oxide materials	ECSA degradation below 10% under FCCJ condition after 10,000 cycles.. 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) and stable operation up to 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)	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