CONCEPT PAPER
for KIER International Cooperation Project

Personal Data	Name of PI	Jeong-gu Yeo	Organization	Korea Institute of Energy Research
	Department	Conversion & Storage Materials Lab.	Title	Principal researcher
	Cell Phone #	010-9760-6592	E-mail	jgyeo@kier.re.kr
Title	Enhancing linear alpha olefin-paraffin separations using membrane			
1. Needs	● Global linear alpha olefin (LAO) Market growth is uprising (2017-2024 CAGR: 1-octene 3.5 %, 1-butene 4.5%). ● Alpha olefins-paraffins separation/purification cost is about 60% of total production. ● LAO produced after catalytic reaction having not high purity of 40~60% is still requiring separation from mixtures. ● The present classical thermal separation processes are very energy-intensive and large footprint.			
2. Competition	● Compact two-stage membrane processes: (1) linear hydrocarbon separation among the various isomers after catalytic reaction using metal-organic framework (MOF), (2) olefin separation from saturated/unsaturated linear hydrocarbon using facilitated transport membrane (FTM) ● Preparation of well-defined MOF membrane having uniform but tunable pore sizes for molecular sieving effect to achieve high separation factor ● Effective separation of FTM using olefin carrier ● No use of harsh chemical co-solvents or energy extensive phase conversion for distillation/condensation			
3. Approach	● Raise separation factor and flux by developing highly-selective materials ● Enhancement of separation factor by molecular design of MOF to control pore size and pore structure ● Development of stable olefin carrier in polymeric matrix			
4. Benefit	● A compact, economic, eco-friendly membrane process for LAO production process ● Introduction of advanced technology for membrane separation process into the growing LAO technology and market ● Further application is expected in dehumidification of HVAC using MOF membrane			
5. Deliverables	● Key deliverable – 2 publications in high impact (top 10%) journals – Feasibility results regarding LAO purity from 50% to more than 90% (to show separation factor more than 20 for C6)			

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Personal Data	Name of PI	Ji Haeng Yu	Organization	Korea Institute of Energy Research
	Department	Energy Conversion & Storage Materials Laboratory	Title	Principal Researcher
	Cell Phone #	+82(42) 860 3414	E-mail	jhyu@kier.re.kr
Title	Interface engineering for integration of a garnet-based solid electrolyte and a high-voltage cathode for all-solid-state batteries			

1. Needs

● Needs of the project

-By 2030, the Ministry of Environment, Republic of Korea plans to reduce greenhouse gas emissions by 37 percent. To meet this goal, electrification of combustion engine-powered transportations is needed to enable zero-emission vehicles. To this end, batteries with high energy density and safety will play a critical role.

-Electric vehicles that are currently available in the market use conventional lithium-ion batteries. However, Li-ion batteries, although fully optimized, have a generic shortcoming associated with safety due to the flammability of a liquid electrolyte, hindering further technological advance.

-All-solid-state batteries using a non-flammable solid electrolyte have received substantial attention as a next-generation, ultimately safe energy storage platform with the potential for higher energy density.

-While several solid electrolyte materials are proposed, their integration model into a device presents a unique challenge due to the complex electro-chemo-mechanical nature of solid-solid interfaces, delaying the development of the all-solid-cell

2. Competition

● Differences and advantages over the current technologies or approaches

-Sulfides, oxides, and organic crystals are reported as Li solid electrolyte materials to date. Among them, lithium lanthanum zirconate (LLZO), an oxide that has a cubic garnet structure, is considered as the most promising candidate due to balanced properties, i.e., good Li conductivity, wide voltage window, and high chemical stability, compared with sulfides and organic materials.

-Challenges to use LLZO for solid-state batteries lie in its integration processing with a cathode. Since both LLZO and cathode are oxides, high-temperature co-sintering is usually required to ensure physical interfacial coherency. However, this method involves chemical interdiffusion across the interface, degrading overall Li transport, as well as high manufacturing cost.

-To enhance the processability for the cell integration, ceramic-polymer composite is widely adopted, which substantially compromises the Li-ion conductivity and, more critically, energy density of a cell.

- In this regard, the most fundamental and desirable approach will be an all-ceramic processing route, but at the lowest possible temperature, that can later employ multilayer ceramic capacitor (MLCC) and low-temperature co-fired ceramics (LTCC) technologies. Key to success in this approach is to develop sintering additives and associated processing technologies that can reduce and synchronize the processing temperature of LLZO and cathode materials.

3. Approach	● Barrier(s) to tackle and how to solve the barriers –This project aims to design multifunctional sintering additives that can be used to co–sinter LLZO and a cathode at low temperature. The additive content and processing conditions will be engineered to suppress interfacial degradation and retain Li ionic conductivity of LLZO. We will also investigate the structure–property relationships of interfaces in LLZO–cathode bilayer samples using electrochemical impedance spectroscopy and electron microscopy. –First, we will design additive ceramics that promotes liquid–phase sintering and investigate processing conditions to achieve crack–free and dense LLZO–cathode bilayer pellets. Ideal additives in our design are expected to reduce the co–sintering temperature below 800°C and preserve the pristine electrochemical properties of LLZO and a cathode. The additive composition will be Li–rich and elements that are redox–inert, such as phosphate and silicate. We also intend to make the additive multifunctional, not only promoting the co–sintering but also passivating some interfaces upon recrystallization. Thus, designed additive material will play multiple roles in the co–sintering process as a sintering aid, mechanical adhesive, and chemical stabilizer. –Second, to estimate the effectiveness of designed sintering additives, we will perform X–ray diffraction (XRD) and transmission electron microscopy (TEM) to uncover interface reactions between LLZO and a cathode upon heat treatment. We will use ex situ XRD and TEM in–house, but for XRD in situ synchrotron resources at Brookhaven National Lab can be accessed if needed. We will optimize the additive content and the heat treatment protocol to obtain coherent interfaces without chemical degradation. –Third, we will assemble an LLZO solid–state cell using the Li metal anode and evaluate battery performance by galvanostatic charge/discharge, cyclic voltammetry, impedance spectroscopy.
4. Benefit	● What is the actual benefits expected from the project –We will find a new additive composition and co–sintering technique that can enable all–ceramic processing in the development of solid–state batteries scalable by multilayer tape–casting. –By stabilizing complex interfaces at low processing temperature, this project will improve fabrication efficiency and cost of all–solid–state batteries. –This research will make us a global leader in the field of all–ceramic battery processing and manufacturing, while most of solid–state battery research has yet focused on properties at a material level, shaping the sustainable energy future.
5. Deliverables	● Key deliverable –Publishing high impact factor journal(1) and International patent(1)

CONCEPT PAPER
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	Department	Ulsan Advanced Energy Technology R&D Center	Title	Senior researcher (Ph.D.)
	Cell Phone #	+82-10-5153-4273	E-mail	jh.oh@kier.re.kr
Title	Investigation on perovskite/silicon heterojunction (SHJ) tandem solar cells made with thinner wafers			
1. Needs	● Perovskite-based tandem approaches are of considerable technological importance to overcome the potentials of high-performance perovskite or c-Si solar cells. ● To realize Perovskite-based tandem cell's full potentials and widen its application areas (e.g. for solar driven electrolysis and self-charging power unit applications), bottom cells made with c-Si wafers need to be made with thinner wafers for reducing materials consumption/cell weight, more mechanically flexible characteristics, and higher open circuit voltages (V_{oc}). • Currently, wafer thicknesses for bottom cells are rather thick, e.g. around 250 μm. (Lang *et al.* Joule (2020), Mazzarella *et al.* (2019), Bittkau *et al.* (2018))			
2. Competition	● To meet the above-mentioned needs, making c-Si bottom cells with thinner wafers may be more productive when adopting SHJ architectures due to its more symmetric structures and low-temperature fabrication processes. ● With the conventional wafer production technologies such as Czochralski/float-zone ingot growth combined with wire sawing processes, there currently exists practical limits for reducing wafer thickness, and this can be overcome by epitaxial wafer growth.			
3. Approach	● With the current wafer production technologies, there exists technological barriers for making thinner wafers due to wire pairing (Ryningen *et al.* (2020)). To tackle these barriers, alternative technologies for making thinner wafers need to be investigated. ● First one might be mechanical and/or chemical thinning methods such as mechanical grinding, CMP, dry etching and/or wet chemical etching. ● Second one is by kerfless wafering, namely by chemical-vapor deposition of epitaxial wafers on porous silicon/parent substrate structures followed by exfoliation. Expecially, this kerfless direct gas-to-wafer technologies can be beneficial for controlling wafer thicknesses simply by varying deposition time. ● In addition, high-efficiency perovskite top cells need to be formed on the textured or flat top surface of thinner symmetrically-structured SHJ bottom cells without inducing any materials defects by further optimizations of coating parameters.			
4. Benefit	● By investigating SHJ bottom cells with thinner wafers for perovskite-based tandem solar cells, one can identify limiting factors and potentials of SHJ bottom cells with thinner wafers, thus leading to optimization of perovskite/SHJ tandem solar cells with thinner wafers. ● Thinner wafers grown with CVD epitaxial growth enables kerfless wafering and also easier thickness and doping density control over the large area, thus paving the way for higher-yield, high-quality and cost-effective thinner wafers for perovskite-based tandem applications.			
5. Deliverables	– Fabrication of epitaxially grown kerfless n-type silicon wafers with thicknesses in the range of 40-200 μm (at least 3 different thickness samples need to be shown by cross-sectional SEM images) * resistivity: in the 0.5 to 20 ohm-cm range – Comparison of measurement results of fabricated lab-scale perovskite/SHJ tandem solar cells made with commercially avaliable (ref.) and thinner (at least with 3 different thicknesses) wafers – at least 1 joint submission and publication for one of SCI(E) journals			

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Personal Data	Name of PI	Jong-Eun Hong	Organization	KIER
	Department	Fuel Cell Laboratory	Title	Principal Researcher
	Cell Phone #	+821030574235	E-mail	jehong@kier.re.kr
Title	Development of protonic conduction fuel cells (PCFCs) adopting an on-cell CO_2 dry reforming of CH_4			
1. Needs	● Securement of a PCFC power generation technology able to combine with a gasification of municipal solid waste (Waste to Energy) ● Reduction of greenhouse gas emissions (CO_2 & CH_4) accompanied by power generation and energy efficiency maximization			
2. Competition	● Capability of directly utilizing a low quality heat energy (500-700°C) and exhaust gases (CH_4, CO_2 & CO) generated by a gasification process ● Application of direct CO_2 dry reforming of methane (CO_2-DRM) as a fuel processing in a PCFC, whose operating cost is 20% lower than steam reforming or partial oxidation			
3. Approach	● Upon the on-cell CO_2-DRM over Ni-based catalysts, severe performance degradation owing to carbon deposition and coarsening of Ni catalyst ● Development of an intelligent non-noble transition metal (TM) catalyst decorated on stable perovskite supports for the CO_2-DRM, which is free of the degradation ● Exsolution technique to produce nano-sized active TM catalyst particles embedded in the support surface, which enhances DRM and prevents the catalyst degradation ● Direct utilization of the catalyst layer developed onto the fuel electrode of PCFCs			
4. Benefit	● Securement of a smart reforming catalyst capable of expanding fuel flexibility in PCFCs ● Confirmation of a complex power generation technology in combination with fuel cell and waste gasification process			
5. Deliverables	● Key deliverable – Conversion of CH_4 & CO_2 85% to 90%, H_2 & CO selectivity 90% to 95%, PCFC power density 〉 0.5W/cm^2, PCFC degradation 〈 1%/kh – Two SCI papers (IF 〉 5) and a patent applied for			

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Personal Data	Name of PI	Rak-Hyun Song	Organization	Korea Institute of Energy Research
	Department	Fuel Cell Laboratory	Title	Principal Researcher
	Cell Phone #	010-3466-0844	E-mail	rhsong@kier.re.kr
Title	Design Flexibility and Manufacturing Reliability with 3D Printing for solid oxide fuel cell			
1. Needs	● Improve the AFL (Anode Functional Layer), electrolyte densities by controlling the interior of the support (enhanced porosity), the distribution of external pores (tightness) using 3D Printing. ● Develop the cell using 3D printing technology which has many advantages, such as, having uniformity of the support and decreasing stress distribution.			
2. Competition	● New and innovative 3D Printing technology: Uniformity of the support will be adopted and the defect occurrence rate will be decreased which provide a great deal of cell performance and leads to SOFC technology commercialization in a market in a near future.			
3. Approach	● Develop green filaments and feedstock for highly filled ceramic powder-polymer mixtures. ● Apply the Fused Deposition Modeling (FDM) for printing highly filled polymer-ceramic powder filaments. ● Produce unique geometric capabilities: Lattice structure for light-weighting. ● Analyse the sintering modeling for densification mechanisms, grain grwoth, pore evolution, and shape distortion.			
4. Benefit	● Enhanced research-based knowledge development will lead more commercialization of a fuel cell technology and provide cost effectiveness of renewable energy. ● Like EV market lead by Tesla, the fuel cell market can be lead by 3D Printing technology.			
5. Deliverables	● Key deliverable – Cell area : more than 10 cm^2, Power density : more than 100 mW/cm^2, Cost down: 20%/kW, CO_2 emission abatement 30% – 2 Publications and 1 Patent			

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	Department	Future Energy Research Division	Title	Principal Researcher
	Cell Phone #	010-6868-5177	E-mail	foifrit@kier.re.kr
Title	Durable hydrocarbon ionomers designed and optimized by developing neural network potential (NNP) for energy conversion systems with anion conducting polymer electrolyte (ACPE)			
1. Needs	● Energy conversion system with ACPE is an attractive technology for low cost hydrogen production due to use of low cost core materials but currently lacks commercially available ionomer ● Currently investigated ionomers suffer from catalytic efficiency loss caused by adsorption of polymer electrolyte ionomer on the electrocatalyst surface ● There is a limit on improving performance and durability of ionomers by current empirical trial-and-error approach ● Theoretical approaches are essential for productivity reducing time and cost occurred by experience approaches			
2. Competition	● Overcoming traditional limitations of computational approaches in research field of polymer science ● Artificial Intelligence (AI)-based machine learning (or deep learning) method is able to simulate big size system with chemical reactions which have remained unsolved until now			
3. Approach	● Investigating chemically optimized ionomers through Density Functional Theory (DFT) calculation ● Training DFT dataset via AI technology and conducting Monte Carlo and molecular dynamics simulation with NNP ● Validation of experimental tests and the analysis of computational feedback in turn will further update the predictive models ● Synthesis of targeted hydrocarbon ionomers and evaluating their surface adsorption behavior with catalyst			
4. Benefit	● Offering high performance ionomer materials as a commercial product ● Offering highly efficient and cost effective new ionomer material discovery platform applicable to energy harvesting systems			
5. Deliverables	● Key deliverable – Ionomer concentration: 〉 15 % in mixed solvents – Ionomer properties Ion exchange capacity: 〉 1.7 meq./g, OH^- conductivity: 〉 0.5 S/cm at 70 °C, Current density stability: 〉 300 h – developing ML force field: 〉 4 elements – simulating atoms number: 〉 2,000 – 2 Journal publications within Top 5% related field			

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Personal Data	Name of PI	Chan Young Park	Organization	Korea Institute of Energy Research
	Department	Greenhouse Gas Research Laboratory	Title	Principal Research Scientist
	Cell Phone #	81-10-5520-9202	E-mail	cpark@kier.re.kr
Title	Reduction of Water Soluble Organic Species using Composite Materials			
1. Needs	Scientists are on a continuous quest to discover increasingly efficient water purification systems under environmentally friendly conditions without requiring expensive energy input. This is because persistent and common organic contaminants including phenol derivatives, nitro compounds, and dyes are one of main global problems to secure safe water. In this sense, **green and energy efficient catalysts** along with membrane-based filtration systems should be developed for water remediation.			
2. Competition	Decontamination of polluted water via common filtration systems: -$100K for 10-20 gal/min micro-(MF) and ultrafiltration (UF) systems -$60K for 5-10 gal/min nano- (NF) and reverse osmosis (RO) systems -$500K~1.5M for 150,000 gal/min wastewater by chelating agents and sedimentation Efficient reduction of water soluble toxic compounds can greatly improve the performance of the above filtration systems Developing a strategy to maximize the advantages of catalytic systems can be utilized in various chemical reactions			
3. Approach	Physical incorporation of reactive metal catalysts into solid materials *in situ* can maintain their original key functions and even possess new physiochemical properties. These materials will be tested as catalysts in chemical reactions associated controlling water quality in conjunction with the treatment of commercially available membranes. The improved catalytic conversion of polluted water will be thoroughly evaluated to develop industrially viable systems at lower cost.			
4. Benefit	Decontaminate and detoxify polluted water Improve water quality via a green and high energy efficient approach at low cost Apply to various chemical transformation reactions such as C-C bond formations, which are important in the production of pharmaceuticals and organic substances.			
5. Deliverables	Key deliverable - Catalytic efficiency over 90% (current 60-70%) - Cost down (minimum of 20% reduction of total cost) - Recyclability waste control: 10 cycles (currently: 4-5 cycles) - Establishing Green solvent conditions (currently: mostly toxic organic solvents) - Extending the lifetime of membrane systems at least 1.5 times - Publications: minimum of two publications in each year (top 20%)			

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Title	Photocatalytic Gaseous CO_2 Conversion			
1. Needs	● The current state-of-the art system for CO_2 reduction reaction depends on an electrolyte because the corresponding reaction mechanisms are well-documented. However, this requires additional expensive procedures to initiate the reaction because CO_2 gas has to be dissolved into the electrolyte solution. Even after the CO_2 dissolution process, CO_2 tends to bubble out from the solution as pressure and temperature change. Moreover, under the liquid phase reaction system, reactant and product molecules are likely to be close to each other, which causes unwanted reverse or side reactions and thus degrades the overall CO_2 conversion efficiency.			
2. Competition	● To overcome the current technical limitations, new gaseous CO_2 conversion systems, desirably using solar power, have to be designed and developed, and the new systems need to reach at least a 10 terawatt scale to have an impact on the global fuels market.			
3. Approach	● In a bid to realize this unprecedented level of CO_2 fixation using H_2O as electron source, we aim to adopt a scalable nanofabrication of leveraging microsphere lithography, dry etchings, and plasma-enhanced atomic layer deposition (ALD) into the seamless constructions for photocatalytic nanotube arrays, which are designed for gas-phase CO_2 reduction using sunlight and water. Specifically, such arrays should have a large number of ALD-grown core (Co_3O_4) – shell (SiO_2) nanotubes operating as independent photosynthetic units under ambient conditions. The SiO_2 nanoshell serves as a H^+ transmitting and O_2 impermeable membrane to spatially separate H_2O oxidation catalysis by Co_3O_4 inside the tube from CO_2 reduction catalysis by Cu, Ag, Fe, or Co nanoparticles outside the tube. This inherent product separation geometry allows to address long-standing scientific barriers of optimizing the combinations of photoactive materials (thermodynamic efficiency) and minimizing charge transfer losses and unwanted reactions (quantum efficiency) of artificial photosynthetic systems.			
4. Benefit	● The core of this proposed research will therefore garner and harness the collaborative expertise to create innovative artificial photosynthetic units converting CO_2 gas directly into value-added chemicals or fuels in a cost-effective manner.			
5. Deliverables	● Key deliverable – The expected key outcomes are solar-powered gaseous CO_2 conversion systems with 5-10% efficiency. (There is no current efficiency example, because the gas-phase CO_2 conversion systems using sunlight and H_2O have never been made.) – Publications and/or Patents: (1) Inorganic oxide-based core-shell nanotube array concept for separating incompatible catalytic environments while maintaining electronic and protonic contact. (2) Robust ultrathin separation membrane for artificial photosynthesis with precisely tunable electron transfer properties and tight molecular separation capability, which are applicable for other types of catalysis in addition to photosynthetic applications. (3) Solar-driven gaseous CO_2 converters using H_2O as electron source.			