International Institute for Carbon-Neutral Energy Research

Molecular Photoconversion Devices Revised Roadmap

March 2019

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Division Objective

Molecular designing of interface between organic and inorganic materials for increased efficiency of photoconversion devices

- Design of high efficiency, long life solar cells using organic semiconductors from control of interfaces
- Highly efficient photocatalysts based on interface design; Two types of photocatalyst will be developed:

  1)Combination of two semiconductors for increased efficiency of water splitting

  2) Design of organic and organometallic systems for the increased efficiency for hydrogen production and/or CO_2 reduction into solar fuels
- Development of energy conservation devices for decreasing CO_2 formation amount based on interface control

  1) Organic light emitting diode and interface control

  2) Control of surface macromolecular brushes for low friction bearings.

Division Projects (1)

Projects	Objective	Research Efforts	Researchers
Project 1 Organic-inorganic hybrid perovskite solar cell	Development of perovskite solar cells with high efficiency and stability	• Improvement of power conversion efficiency by development of new perovskite and cell structures, interface engineering, and utilization of tandem solar cell structures. • Enhancement of lifetime by optimization of cell fabrication conditions, development of new hole- and electron-transporting materials, analyses of degradation mechanisms, and management of defect levels in film bulks and at interfaces	Adachi, Nakanotani, Goshi, Rockett, Matsushima, ~~Seo~~, Qin, Fujiwara, Leyden
Project 2-1 Hybrid catalyst for Photo water splitting	Water splitting with organic and inorganic composite	Optimized inorganic and organic semiconductor for effective charge separation	Ishihara, ~~Ida, Hagiwara, T.Sakai~~, Staykov. Ertekin, Takahara, ~~Higaki~~, Watanabe~~, Li, Sun, Honda,~~ Lippert, Takagaki, Son, Kosem
Project 2-2 Molecular catalysts for the generation of solar fuels	*Molecular-based photocatalysts for water splitting and/or CO_2 reduction to give solar fuels*	*Fabrication of rapid catalytic cycles for water oxidation and reduction by fine tuning of structural and electronic properties of organometallic frameworks, together with development of efficient photocatalytic systems for solar CO_2 reduction.*	*K. Sakai, K. Yamauchi, H. Ozawa, A. Call, M. Cibian*

Division Projects (2)

Projects	Objective	Research Efforts	Researchers
Project 2-3 Severely-strained and high-pressure compounds for photocatalyst	Development of photocatalysts with high efficiency under visible light using high-pressure torsion (HPT)	Improvement of photolytic activity of inorganic compounds by stabilizing lattice defects and low-bandgap high-pressure phases using severe plastic deformation under high pressure	~~Horita~~, Edalati, Wang, Arita
Project 3-1 Rare-metal-free organic and hybrid perovskite light-emitting diodes	Development of organic and hybrid perovskite light-emitting diodes with high efficiency and stability	• Improvement of external quantum efficiency by development of new materials and device structures and modification of light outcoupling. • Enhancement of lifetime by development of new emitting and carrier-transporting materials and interface engineering.	Adachi, Nakanotani, Goshi, Matsushima, Qin, Leyden
Project 3-2 Surface Molecular Blush	*Development of low friction bearings based on macromolecular blushes*	Design of macromolecular brushes immobilized on metal and carbon fiber reinforced plastics for friction control-surface coating	~~Higaki~~, Takahara, Ertkin, Tanaka, Shundo,

Milestones (1)

	2014-2020 (short)	2021-2025 (mid)	2025-2050 (long)
Project 1: Organic-inorganic hybrid perovskite solar cell	Development of new perovskite and cell structures Power conversion efficiency > 20% **(Accomplished)**	Enhancing interface engineering Power conversion efficiency > 24%	Utilization of tandem solar cell structures Power conversion efficiency > 30%
	Optimization of cell fabrication conditions 50% lifetime > 10,000 h (100 mW/cm^2, AM1.5G solar irradiation) **(Accomplished)**	Development of new carrier-transporting materials and analyses of degradation mechanisms 50% lifetime > 30,000 h (100 mW/cm^2, AM1.5G solar irradiation)	Management of defect levels in film bulks and at interfaces 50% lifetime > 90,000 h (100 mW/cm^2, AM1.5G solar irradiation)

Commercialization of solution-processable perovskite solar cells with high efficiency and stability (advantageous as an alternative technology of widely used silicon-based solar cells in terms of lower-cost solar power conversion)

Milestones (2)

	2014-2020 (short)	2021-2025 (mid)	2025-2050 (long)
Project 2-1: **Hybrid catalyst for Photo water splitting**	Design and synthesis of New Dye (Alene and phosphine) for charge separation	Plate type reactor and light focus rector design	Plate type reactor and applied small potential
	Design and synthesis of Narrow band semiconductor (GaON, InON etc) and dopant for charge separation	Applied nanostructure control for new inorganic semiconductor(nanocube mesoporous etc.)	Long term stability. Combination of Inorganic catalysts and applied heterojunction
	Application of Hydrogenase (Fe-Fe and Fe-Ni), Nitrogenase	Apply new organic dye like organic perovskite and interface control	Long term stability of biocatalyst applied catalyst
		Application of New Enzyme such as cyanobacteria	
	Energy conversion efficiency >1%	Energy conversion efficiency >10%	Energy conversion efficiency >20% Large size unit >100Nm3/h Competitive cost

Milestones (3)

	2014-2020 (short)	2021-2025 (mid)	2025-2050 (long)
Project 2-2: **Molecular catalysts for the generation of solar fuels (H_2, HCOOH, HCHO, CH_3OH, CH_4, CO, etc.)**	Design and Synthesis of New Molecular Catalysts for H_2/O_2 Generation from Water and CO_2 Reduction to Fuels. Preparation of Molecule-Semiconductor Hybrids Photocatalyzing Water Oxidation and Water/CO_2 Reduction to Fuels. Achievement of Practical Models for Solar Fuels Generation. Energy conversion efficiency >1%	Development of Practically Useful Photochemical Systems for Solar Fuels Generation Pursue Possibility of Fabricating Model Systems for Commercial Products under Collaboration with Companies Energy conversion efficiency >10%	Durability Tests towards Improvement in Long-Term Durability of our Individually Developed Model Systems for Wide-Spread Applications in Solar Energy Conversion and Storage. Product Storage and their Commercial Circulation for the Actual Wide-Spread use in Our Society. Energy conversion efficiency >20% Large size unit >100Nm3/h Competitive cost

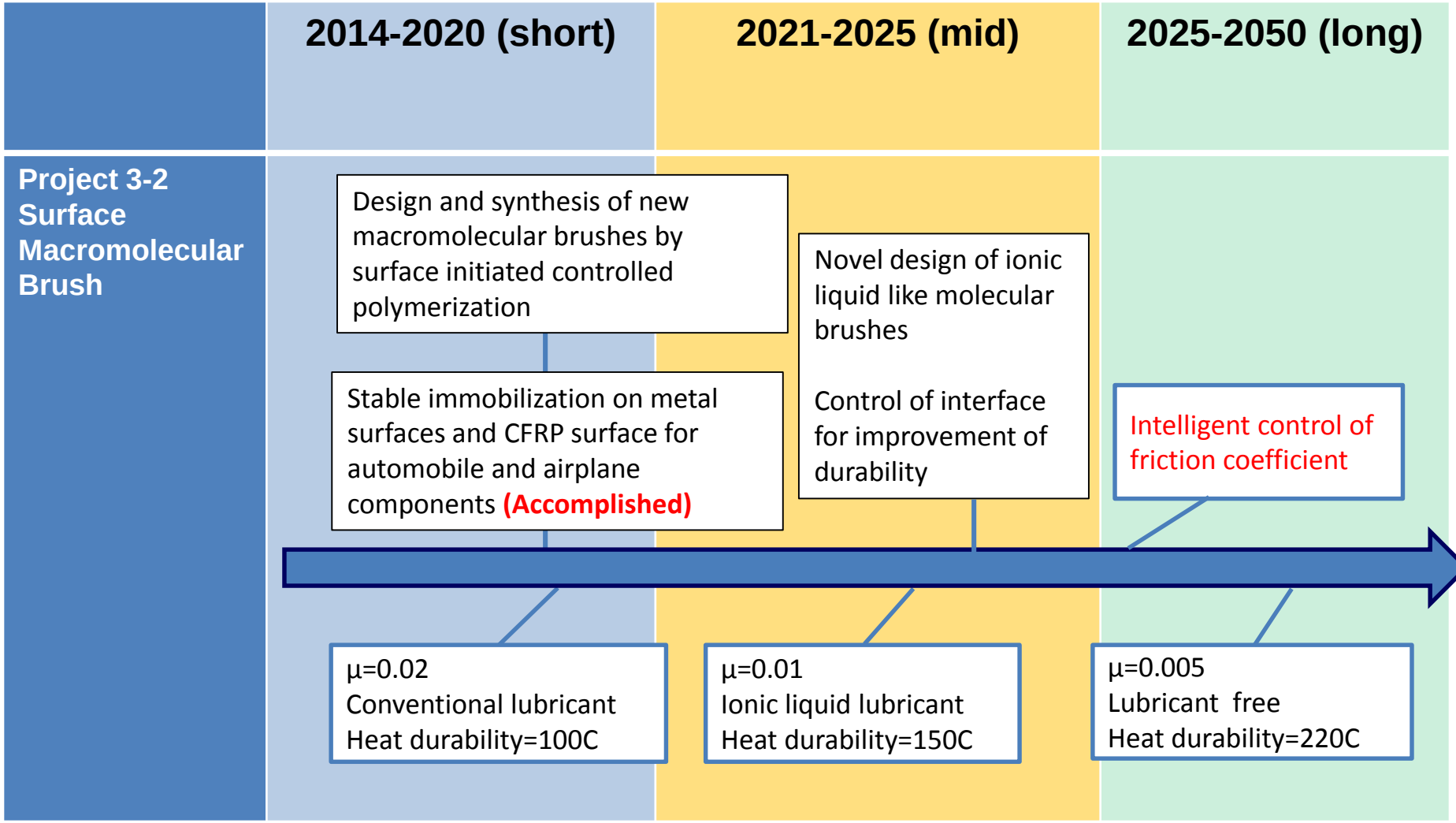
Milestones (4)

	2014-2020 (short)	2021-2025 (mid)	2025-2050 (long)
Project 2-3: **Severely-strained and high-pressure compounds for photocatalysis**	Bandgap engineering of nanostructured TiO_2 and ZnO for visible-light-driven photocatalysis by stabilizing high-pressure phases and oxygen vacancies	Application of high-pressure torsion process to synthesize new severely-strained complex oxides and oxynitrides for photocatalysis with high efficiency	Design new methods to synthesize severely-strained and high-pressure phases at the large scale
	Application of severe plastic strain via high-pressure torsion to enhance photocatalysts from natural minerals and perovskites	Application of metastable high-pressure phases for conversion of CO_2 to fuels by photocatalysis and electrolysis	Stabilize high-pressure phases by composition control
			Expand application of severely-strained and high-pressure phases in nanoionics
	Energy conversion efficiency >1%	Energy conversion efficiency >10%	Energy conversion efficiency >20% Large size unit >100Nm3/h Competitive cost

Milestones (5)

	2018-2020 (short)	2021-2025 (mid)	2025-2050 (long)
Project 3-1: Rare-metal-free organic / hybrid perovskite light-emitting diodes	Development of new materials and device structures External quantum efficiency > 40% (with out-coupling) Power conversion efficiency > 70 lm/W **(Accomplished)**	Modification of light out-coupling External quantum efficiency > 60% Power conversion efficiency > 130 lm/W	Commercialization of highly efficient, stable organic and perovskite light-emitting diodes (advantageous over existing display and lighting technologies based on liquid crystals, inorganic light-emitting diodes, etc. in terms of low-carbon-emission manufacturing and low power consumption)
	Development of new emitting materials 50% lifetime > 10,000 h (initial luminance: 3,000 cd/m^2) **(Accomplished)**	Utilization of new carrier-transporting materials 95% lifetime > 50,000 h (initial luminance: 3,000 cd/m^2)	Enhancing interface engineering 95% lifetime > 100,000 h (initial luminance: 3,000 cd/m^2)

Milestones (6)



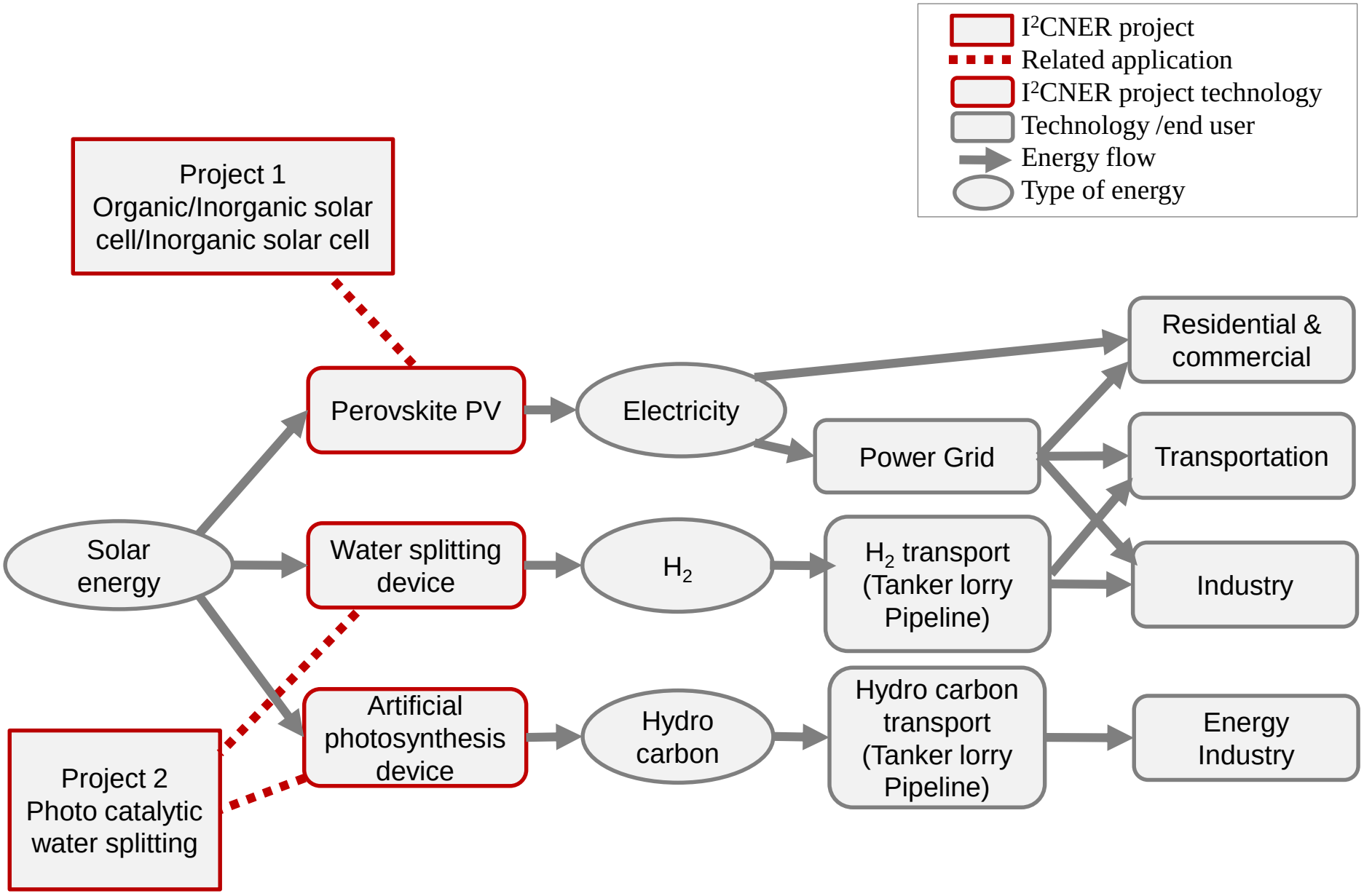
Ultimate Targets

	Ultimate targets	Current Benchmarks	Technology/ Application
Project 1 Organic/inorganic hybrid perovskite solar cell	• Power Conversion Efficiency >30% • 50% Lifetime > 90000 h	• Certified Maximum Power Conversion Efficiency = 23.7% (KRICT)	• Stable and high efficiency PV based on perovskite structure
Project 2 Photo catalytic water splitting	• Energy conversion efficiency >20% • Large size unit >100Nm^3/h • Competitive cost <20 yen/m^3	• Efficiency=1.1% • Durability is low Sheet catalyst Domen et al.	• Device to produce hydrogen using solar energy • Device to convert CO2 to hydrocarbon using solar energy
Project 3-1 Rare-metal-free organic and hybrid perovskite light-emitting diodes	• External Quantum Efficiency > 60% • Power Conversion Efficiency >130 lm/W • 95% lifetime >100,000h • Low cost	• External quantum efficiency = 30% Kaji et al	• High efficiency and long life LED and lightening device
Project 3-2 Surface Molecular Brush	• μ=0.005 • Lubricant free • Heat durability=220C	• μ=0.1(Gel coat) Wada et al (low heat stability ~50C)	• Bearing with high efficiency (e.g. lubrication in automobile) • Anti-marine fouling for marine shipping industry • Anti-icing for aeronautical application

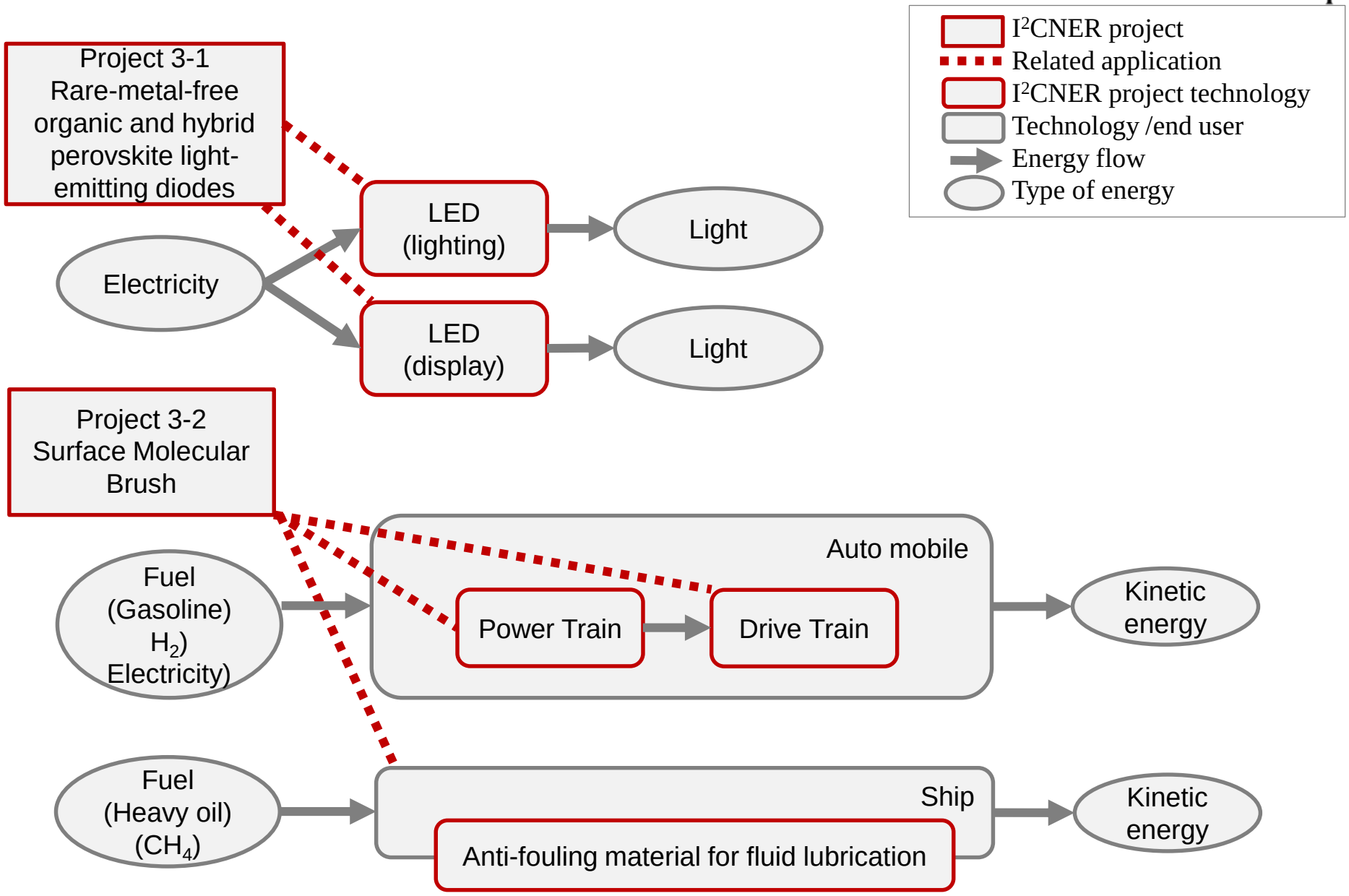
Role & Contribution through Technology

- The role of this division toward CNS is to create:
  1. stable and high efficiency, low cost PV based on perovskite structures, contributing to the deployment of PV and providing cheap low carbon electricity
  2. devices to produce hydrogen (water splitting) using solar energy and devices to convert CO_2 to hydrocarbons (artificial photosynthesis) using solar energy, contributing to providing cheap low carbon hydrogen and carbon neutral hydrocarbons
  3. high efficiency and long life LED and lighting devices to save energy in lighting applications
  4. efficient lubrication and anti-fouling system to save energy in various appliances such as the automobile

Technology/Application (1)



Technology/Application (2)



Note: these are two examples of the application of Project 3-2