



PHYSICAL AND LIFE SCIENCES DIRECTORATE
MATERIALS SCIENCE DIVISION

KIST-LLNL Workshop

September 23-26, 2019

September 23, 2019

8:00 a.m.	Registration and Light Breakfast	Bldg. 6475 (HPCIC)
8:30 a.m.	Welcome and Meeting Objectives	Yong Han Group Leader Materials Science Division, LLNL
8:45 a.m.	Welcome	Pat Falcone Deputy Director for Science and Technology, LLNL
9:00 a.m.	Overview of Physical and Life Science Directorate	Glenn Fox Associate Director, Physical and Life Sciences, LLNL
9:20 a.m.	Material Science Division Capabilities and Highlights	Bob Maxwell Division Leader, Materials Science Division, LLNL
9:40 a.m.	Korea Institute of Science and Technology (KIST) Overview	Seok Jin Yoon Vice President, KIST
10:00 a.m.	Break	
10:10 a.m.	Group Photo	
10:20 a.m.	Materials for Energy at LLNL	Tony Van Buuren Deputy Division Leader, Materials Science Division, Associate Program Leader, LLNL
10:40 a.m.	HyMARC and HydroGEN Programs at LLNL	Brandon Wood Staff Scientist and HyMARC Lead

Technical Contact: Yong Han, 925.423.9772, han5@llnl.gov
Administrative Contact: Tara Ruchonnet; 925.423.2167; ruchonnet3@llnl.gov
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Release Number: LLNL-MI-789682



11:00 a.m.	Research Activities at the Center for Energy Materials	Ji-Won Son Center for Energy Materials Research, KIST
11:20 a.m.	Research Activities of Center for Energy Storage Research at KIST	Kyung Yoon Chung Center for Energy Storage Research, KIST
11:40 a.m.	Introduction of KIST Hydrogen and Full Cell Research	Chang Won Yoon Center for Hydrogen and Fuel Cell Research, KIST
12:00 p.m.	Lunch and Badge Pick-Up	Westgate Badge Office
2:00 p.m.	Breakout Session Directions	
2:10 p.m.- 5:00pm	Breakout Sessions Group #1 Yosemite Room Hydrogen Storage, Production, and Fuel Cells Group #2 Appalachian Room All-Solid State Batteries Group #3 Acadia Room Data Science Group #4 Denali Room Characterization Group #5 Collaboration Area R&D Planning and Staff Evaluation	
	Group 1 – Hydrogen Storage, Production, and Fuel Cells Discussion Leads: Ji-Won Son and Brandon Wood	
	Hydrogen production from formic acid and formate for fuel cells	Hyangsoo Jeong Senior Researcher, Center for Hydrogen and Fuel Cell Research, KIST
	Solid state hydrogen storage research in KIST	Young-Su Lee Principal Researcher, Center for Energy Materials Research, KIST
	LLNL's modeling activities for HyMARC	ShinYoung Kang Staff Scientist, Quantum Simulation Group, LLNL
	Manufacturing Molecules for the Carbon Economy	Eric Duoss Group Leader, Advanced Materials, Manufacturing & Processing Technologies

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LLNL's modeling activities for HydroGEN

Tuan Anh Pham
Staff Scientist, Quantum Simulation
Group, LLNL

Intermediate temperature fuel cell membrane

Patrick Campbell
Staff Scientist, Advanced Materials
Synthesis Group, LLNL

Group 2 – All-Solid State Batteries

Discussion Leads: Kyung Yoon Chung and Tae Wook Heo

Lithium Ion Conducting Oxide $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ for All Solid State Li Batteries

Seungho Yu
Senior Researcher, Center for
Energy Storage Research, KIST

(Tentative) Overview of Solid-state Batter Research at KIST

Kyung Yoon Chung
Head, Center for Energy Storage
Research, KIST

Mesoscale Approach for Modeling Solid-state Electrodes and Electrolytes

Tae Wook Heo
Staff Scientist, Computational
Materials Science Group, LLNL

3D Printing of All-solid-state Lithium Batteries

Jianchao Ye/Marissa Wood
Staff Scientist, Nanoscale
Integration Science Group, LLNL

Atomistic Modeling of Interfaces in Solid-state Batteries

Sabrina Wan
Postdoctoral Research Staff
Member, Quantum Simulation
Group, LLNL

3D Printing and Optimization of Energy Storage Materials

Marcus Worsley
Staff Scientist, Advanced Materials
Synthesis Group, LLNL

Group 3 – Data Science

Discussion Leads: Sang Soo Han and Yong Han

Activities of Multiscale Simulation and Machine-Learning in KIST

Sang Soo Han
Principal Researcher, Computational
Science Research Center, KIST

Machine learning surface interactions to accelerate catalyst discovery

Donghun Kim
Senior Researcher, Computational
Science Research Center, KIST

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Reliable and Explainable Machine Learning

Bhavya Kailkhura
Staff Scientist, Center for Applied
Scientific Computing, LLNL

Group 4 – Characterization
Discussion Leads: Jong Han Song and Graham Bench
(CAMS tour)

Jong Han Song
Principal Researcher, Computational
Science Research Center, KIST

Current status of KIST ion beam accelerator facilities and
AMS researches

Byung-Yong Yu
Researcher, Advanced Analysis
Center, KIST

Graham Bench
Director, CAMS, LLNL

Group #5 R&D Planning and Staff Evaluation
Discussion Leads: Glenn Fox and Jong Joo Kim

5:00 p.m.

Wrap-up and Adjourn

6:00 p.m.

Welcome Dinner hosted by LLNL

Lazy Dog Restaurant
4805 Hacienda Dr.
Dublin, CA 94568

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KIST-LLNL Workshop
Tuesday

September 24, 2019

8:30 a.m.	Light Breakfast	Bldg. 6475 (HPCIC)
9:00 a.m.	Breakout Instructions	
9:10 a.m.	Breakout Sessions	
	Group 1: Hydrogen Storage, Production, and Fuel Cells, Discussion Leads: Chang Won Yoon and Brandon Wood	Group #1 Yosemite Room Group #2 Appalachian Room
	Group 2: All-Solid State Batteries, Discussion Leads: Kyung Yoon Chung and Tae Wook Heo	Group #3 Acadia Room Group #4 Denali Room
	Group 3: Data Science Discussion Leads: Sang Soo Han and Yong Han	
	Group 4: Characterization Discussion Leads: Jong Han Song and Graham Bench	
10:30 a.m.	Break	
10:45 a.m.	Resume Session and Prepare Breakout Report	
12:00 p.m.	Lunch	
1:30 p.m.	Breakout Reports	
3:30 p.m.	Break	
4:00 p.m.	Discussion	
5:00 p.m.	Wrap-up and Adjourn	
6:00 p.m.	Thank You Dinner hosted by KIST	

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KIST-LLNL Workshop

Wednesday

September 25, 2019

9:00 a.m.	Tours		Bldg. 6475 (HPCIC)
		Chris Spadaccini, AML Chris Spadaccini, Additive Manufacturing Fred Holdener, NIF Tour Jeremy Feaster, Synthesis and Characterization Tours	
12:00 p.m.	Lunch		
1:30 p.m.	Mini-Breakout Sessions		
5:00 p.m.		Group 1: Hydrogen Storage, Production, and Fuel Cells	Group #1 Yosemite Room
		Group 2: All-Solid State Batteries	Group #2 Appalachian Room
		Group 3: Data Science	Group #3 Acadia Room

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Agenda Date: DRAFT – September 10, 2019

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KIST-LLNL Workshop

Thursday

September 26, 2019

9:00 a.m.	Mini-Breakout Sessions	Bldg. 6475 (HPCIC)
	Group 1: Hydrogen Storage, Production, and Fuel Cells	Group #1 Yosemite Room
	Group 2: All-Solid State Batteries	Group #2 Appalachian Room
	Group 3: Data Science	Group #3 Acadia Room
12:00 p.m.	Adjourn	

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