

Challenge Program **Materials for Clean Fuels**

Phil De Luna
Program Director

1916 CANADA EVOLVES - THE NRC RESPONDS TODAY

NATION BUILDING	WAR TIME	BOOM TIME	SPACE RACE	DIGITAL + GLOBAL	CLIMATE CHANGE
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Advice

1928 Conduct applied and industrial R&D

1946 Conduct basic science, provide support for small and medium-sized enterprises (IRAP)

1986 Industry-oriented institutes

2000 Regional expansion and cluster initiatives

2012 Research and Technology Organization (RTO)

2016 + Renewed focus on excellence and engagement

2020 COVID-19

EVOLVING
NRC ROLE



173

buildings
located on

22

sites

564,000 m²

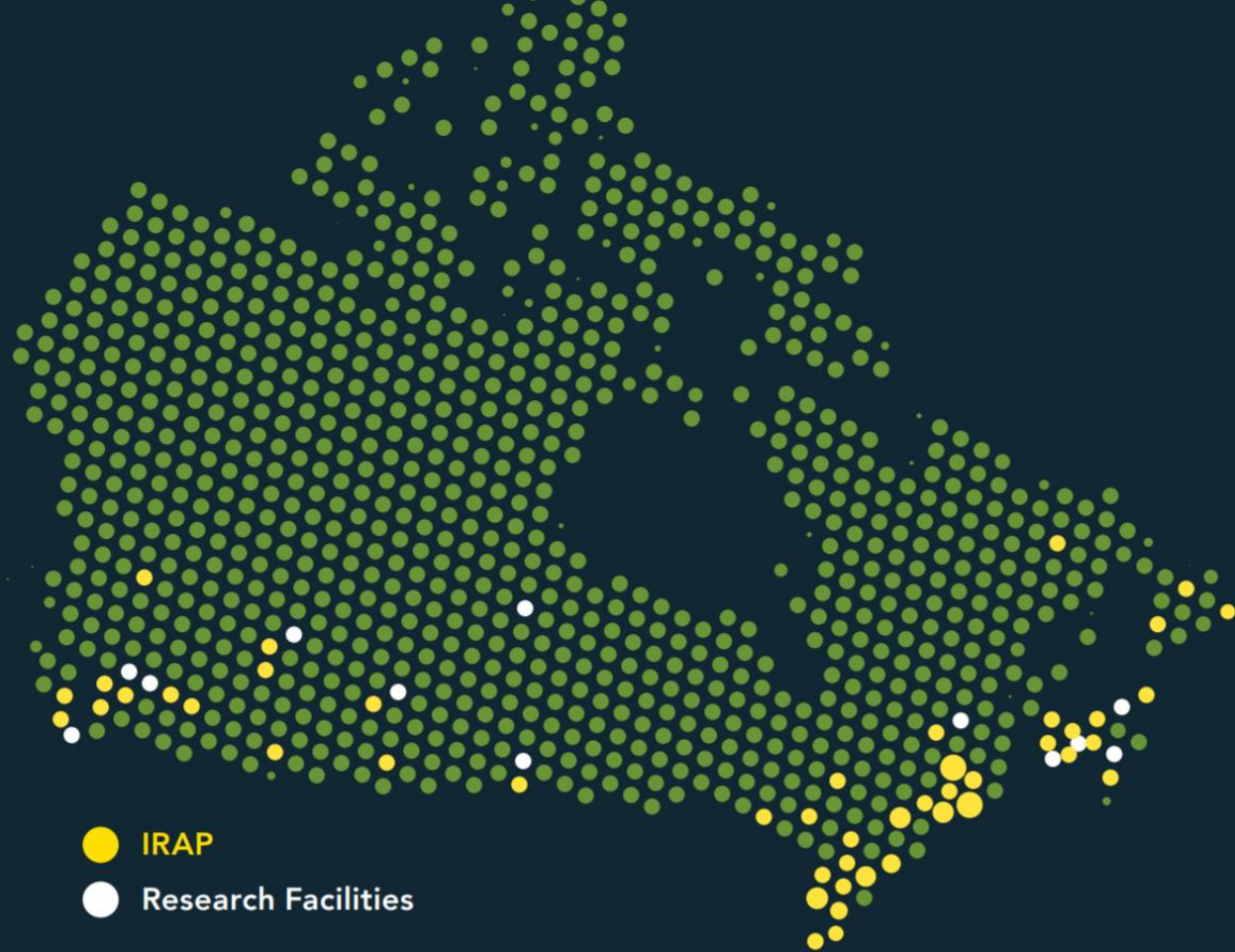
of NRC facilities
across Canada

3,700

scientists, engineers,
technicians and other
specialists, including

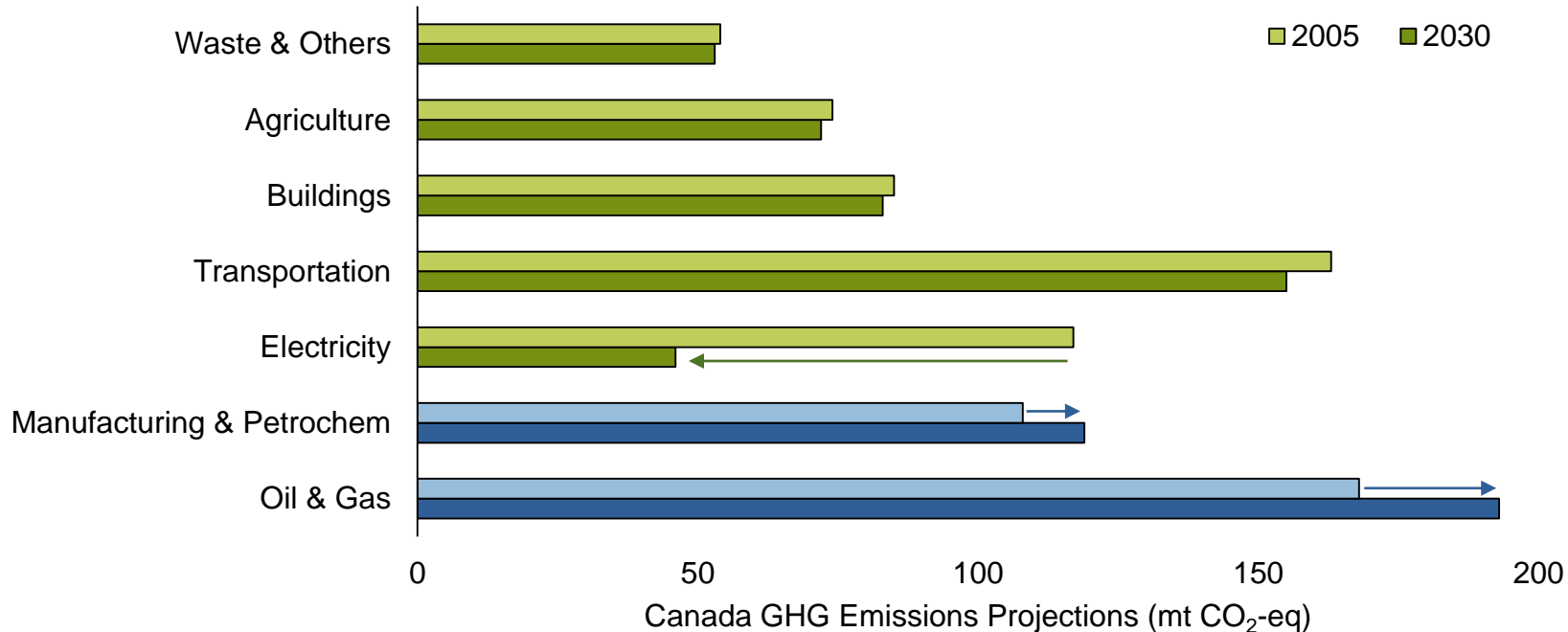
255

industrial
technology
advisors



Our Challenge

Develop **novel materials** needed for **clean energy systems** to meet Canada's **emissions reductions** commitments at **low cost**



Our 2050 Target



2007

2016

2019

65% GHG
reduction
by 2050

80% GHG
reduction
by 2050

100% GHG
reduction by
2050

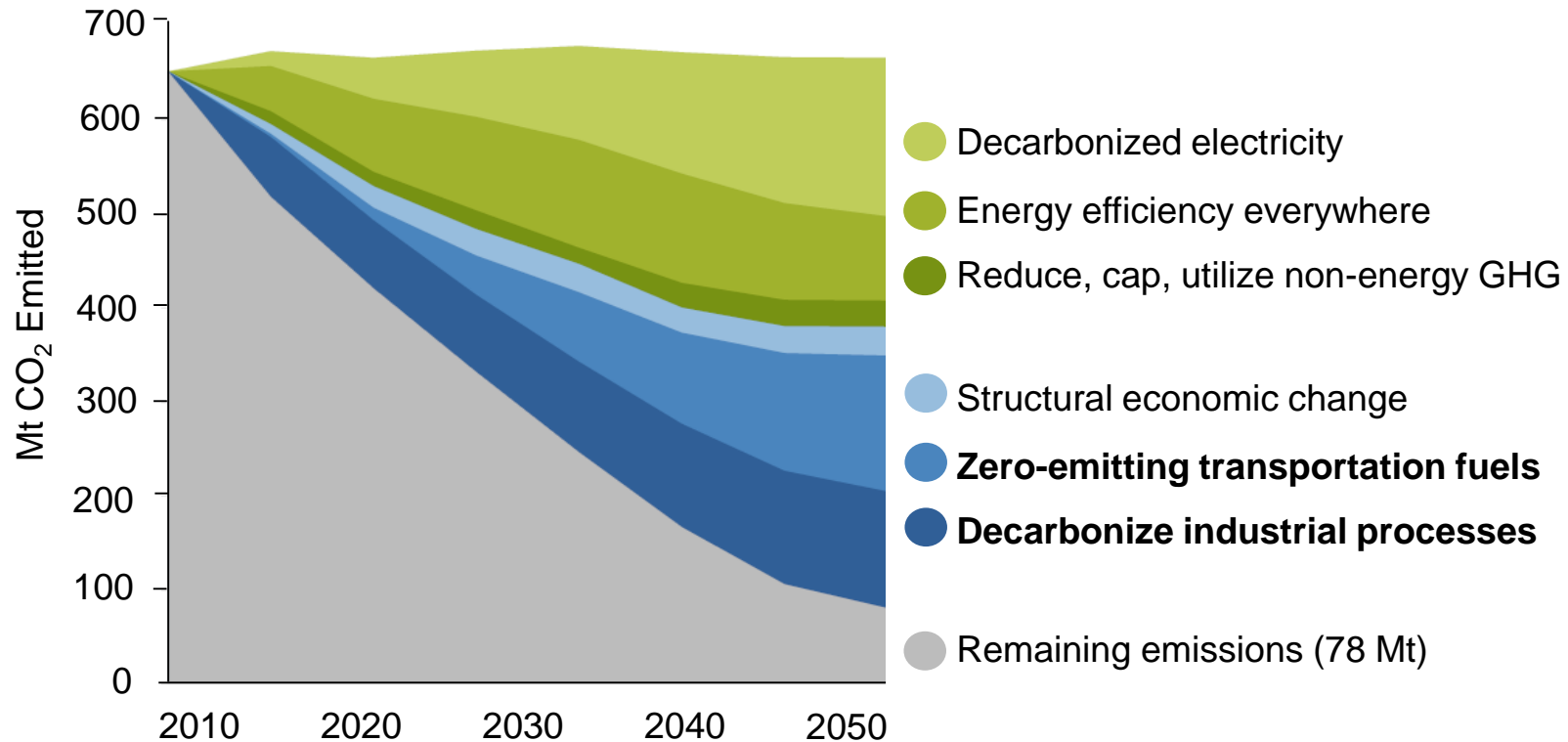


€9 billion long-term renewable hydrogen strategy

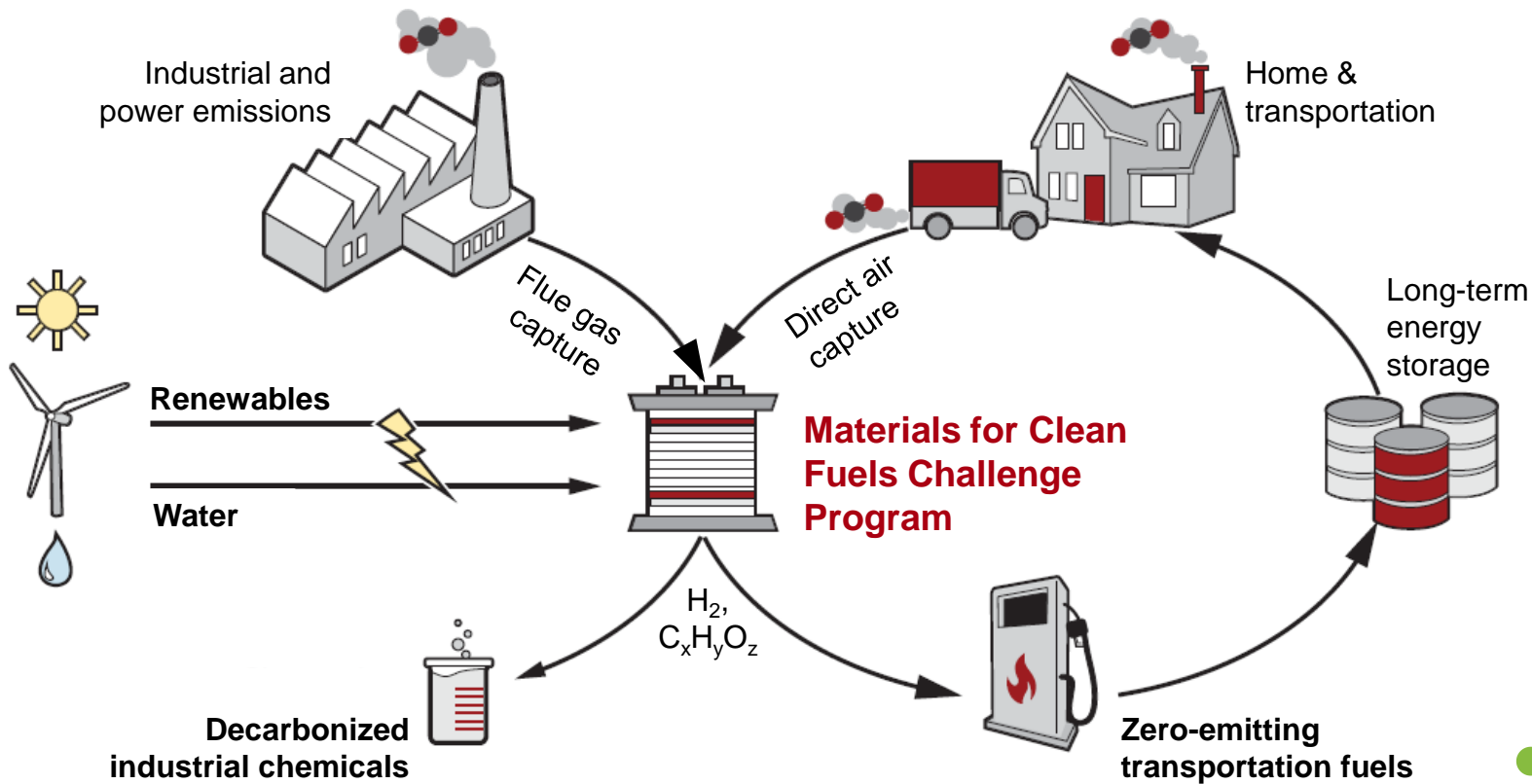


€100 million for innovation in CO₂ direct air capture

Pathways to Decarbonize Canada



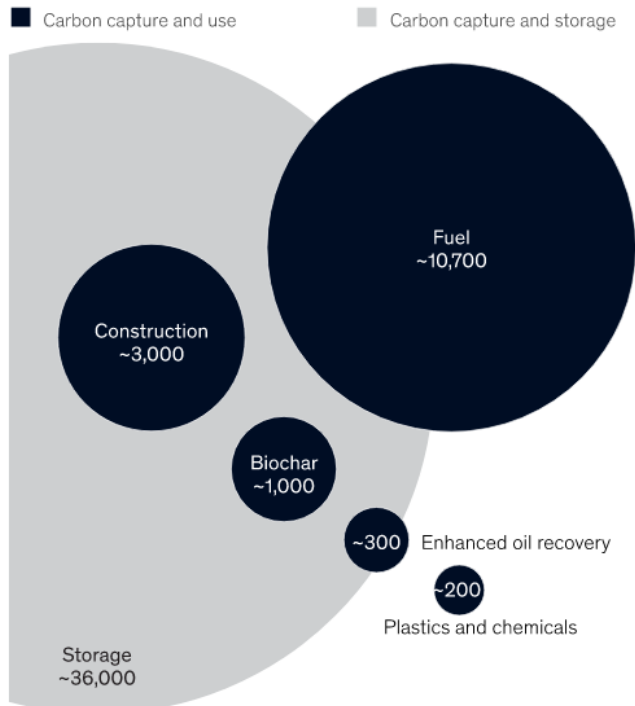
A Renewably Powered Chemical & Fuels Industry



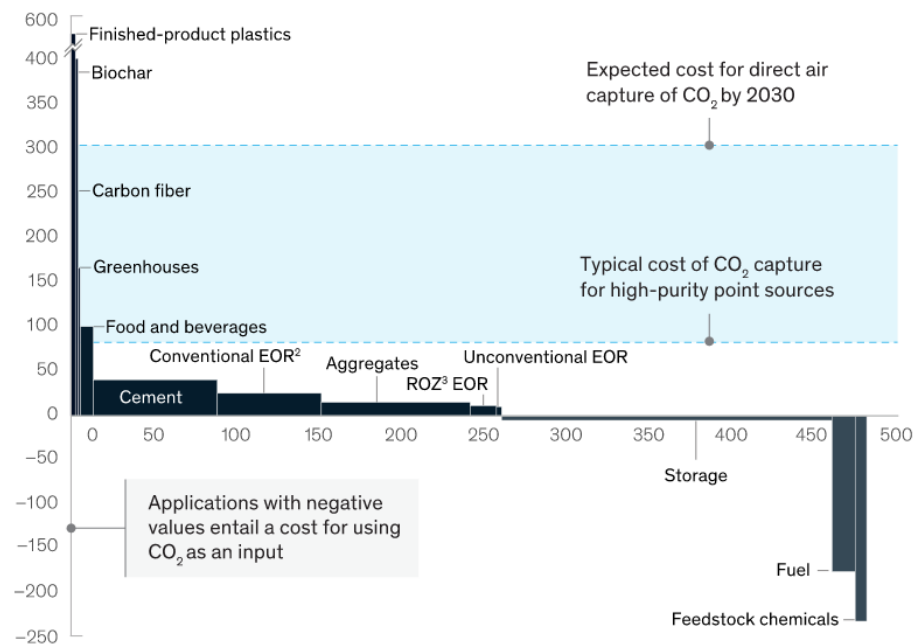
Converting CO₂ Into Renewable Fuels and Chemicals

Source: McKinsey, June 30, 2020

Technical potential of CCUS in 2030, metric megatons of CO₂ per






\$ per ton of CO₂



Sequestered CO₂ volume,⁴ 2030 potential, megatons per year

Challenge Program

Goal | Develop innovative materials for renewable fuels & chemical feedstocks

Themes	CO ₂ Conversion 	Industrial H ₂ 	Accelerated Materials Discovery 
	Materials Research & Development	Systems Prototyping & Scale	Technoeconomic Assessment & Commercialization

Outcomes | Economically viable processes for CO₂ conversion, H₂ production and future renewable fuels production

Evaluation | Publications, patents, # HQP, cost reduction against incumbents, spinoff companies, # new materials

Technology Focus Areas & Timeline



**Artificial
Intelligence &
Robotics**



**Catalyst Design &
Synthesis**



**Membrane Design
& Synthesis**



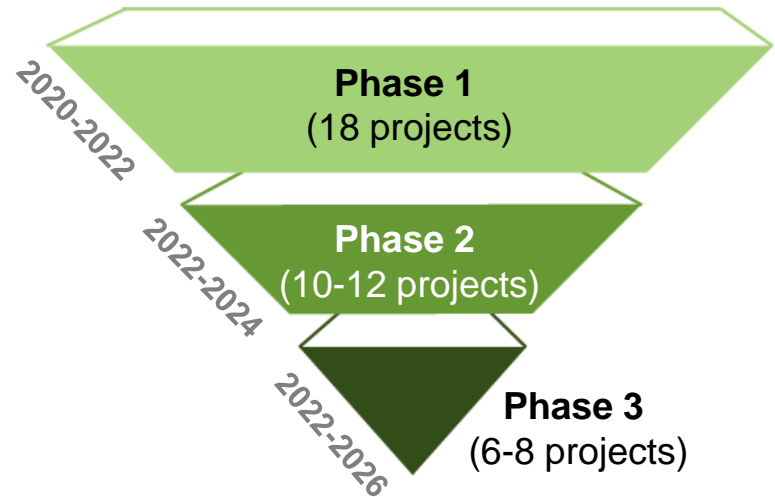
**Device
Incorporation &
Prototyping**



**Characterization &
Spectroscopy**



**Technoeconomics &
Life Cycle**



Who We Are

7 Canada Research Chairs

11 Female Principal Investigators

14 Early Career Researchers

Canadian



International



SMEs



NRC Research Activity to Date

10 Published Journal Articles

\$366K Booked Revenue

\$12M Grants & Contributions Awarded

PERSPECTIVE
nature materials

Molecular enhancement of heterogeneous CO₂ reduction

Dae-Hyun Nam^{1,2}, Phil De Luna^{1,2,3,4,5}, Alonso Rosas-Hernández^{6,4,5}, Arnaud Thevenon⁶, Fengwang Li^{1,2}, Theodor Agapie^{1,4}, Jonas C. Peters^{1,4}, Osama Shekiah⁶, Mohamed Eddas⁶, Edward H. Sargent^{1,2,3,4,5}

The electrocatalytic carbon dioxide reduction reaction (CO₂RR) addresses the need for storage of renewable energy...

APPLIED ENERGY MATERIALS

Bipolar Membrane Electrode Assemblies for Water Electrolysis

Benja Meyerhöfer, David McLaughlin, Thomas Böhm, Manuel Hegelheimer, Dominik Seeburger, and Simon Thiele

ABSTRACT: We present the first analysis of a zero-gap bipolar membrane water electrolysis cell with liquid water. Our electrolysis features a high pH environment for the oxygen evolution reaction and a low pH environment for the hydrogen evolution reaction. The advantages of proton exchange membrane water electrolysis can be combined with those of anion exchange membrane electrolysis by including a water splitting bipolar membrane in the path to a bipolar membrane electrode assembly (BMEA) to investigate the cell operation for the cell performance as the bipolar membrane with and without anion exchange membrane (AEM) and cation exchange membrane (CEM) interface directly between the O₂ and H₂ evolution reactions.

nanomaterials

Three-Dimensional Cathodes for Electrochemical Reduction of CO₂: From Macro- to Nano-Engineering

Shiqiang (Rubi) Hu^{1,2}, Nina Shalagin³, Vladimir Noshchikov³, Lei Zhang³, Kouroush Malek³, Michael Elkering³, and Phil De Luna⁴

ABSTRACT: Rising anthropogenic CO₂ emissions and their climate warming effects have triggered a global response in research and development to reduce the emissions of this harmful greenhouse gas. Electrochemical CO₂ reduction (CO₂RR) is a promising technology to convert CO₂ into value-added products, but industrial deployment. This work delivers studies of three-dimensional cathodes for CO₂RR. The fabrication of three-dimensional cathodes for high-performance CO₂RR is discussed.

PHYSICAL REVIEW E 101, 052604 (2020)

Learning to grow: Control of material self-assembly using evolutionary reinforcement learning

Stephan Whitlam¹
Molecular Foundry, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, California 94720, USA

Isaac Tambly^{2,3}
National Research Council of Canada, Ottawa, Ontario, Canada
and Vector Institute for Artificial Intelligence, Toronto, Ontario, Canada

(Received 29 December 2019; revised manuscript received 10 February 2020; accepted manuscript online 10 February 2020)

ChemRxiv

Virtual Materials Intelligence for Design and Discovery of Advanced Electrocatalysts

Ali Malek^{1,2}, Mohammad Javad Estamizad^{1,2}, Mehrdad Mokhtari^{1,2}, Qiang Wang^{1,2}, Michael H. Elkering^{1,2}, and Kouroush Malek^{1,2,3}

Similar to autonomous general from big data in genomics, security, internet of things, and e-commerce, the materials work flow can be made more efficient and precise through advances in assembling data sources, autonomous material synthesis, rapid characterization, big data analytics, and self-learning algorithms. In electrochemical material context, data sets are large, structural heterogeneity, and difficult to process and analyze from a single data channel or platform. Computer-aided material design together with advances in data mining, machine learning, and predictive analytics are required to process, interpret and predict the materials properties for CO₂ conversion in a use case.

ChemRxiv

Development of Fukui Function Based Descriptors Learning Study of CO₂ Reduction

Sergey Gusakov¹, Stanislav R. Stoyanov, and Samira Siahrostami

ABSTRACT: Developing novel methods that capture chemical properties quickly and with reasonable accuracy has emerged as an attractive way to replace time-consuming density functional theory (DFT) calculations. In this study, we propose a new type of machine learning (ML) enhanced descriptors based on the Fukui function (FF) projected onto the Cominsky surface. The FF contains information about the local system's response to the perturbation and could be used as a descriptor of the chemical properties of a surface. We show that the FF, augmented by a general characteristic of the electronic structure of the surface, such as a work function, is well correlated to the measured adsorption energy of CO₂. Therefore, this combination might replace the computationally expensive mapping of the adsorption energy of small molecules as an indicator of catalytic activity. Potential extensions of the proposed methodology are briefly discussed.

Matter

Crystal Site Feature Embedding Enables Exploration of Large Chemical Spaces

Heath Choudhry, Mikael Anders, Kevin Rykacz, Christian Wang, Ali Malek, Isaac Tambly, Edward H. Sargent

ABSTRACT: The representation enables efficient and targeted exploration of chemical spaces. It provides a generalization of chemical space beyond those used in the training process. It is built on a hierarchical power-law representation of chemical space.

APPLIED ENERGY MATERIALS

Development of Fukui Function Based Descriptors Learning Study of CO₂ Reduction

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ChemRxiv

Combined energy storage and methane bioelectrosynthesis from carbon dioxide in a microbial electrosynthesis system

Abdullah Gonen Vidale¹, Susha Oommen¹, Boris Tarkenton^{1,2}

ABSTRACT: Microbial electrosynthesis (MES) is a promising technology for the production of value-added chemicals and fuels from CO₂. However, the low efficiency of MES is a major challenge. In this study, we propose a combined energy storage and methane bioelectrosynthesis system. The system consists of a microbial electrosynthesis system (MES) coupled with a microbial fermentation system (MFS). The MES produces H₂ and the MFS produces CH₄. The H₂ is then used for the bioelectrosynthesis of CH₄. This system shows a significant improvement in the efficiency of MES compared to the conventional MES system.

CO₂ Conversion Projects

Electrocatalytic

- Anion exchange membranes for CO₂ conversion (**Ionomr / Simon Frasier University**)
- High-temperature SOECs for CO₂ conversion to methane (**University of Toronto**)
- In-situ and operando characterization of CO₂ electrocatalysts (**McMaster**)
- Direct conversion of CO₂ from direct air capture solutions (**University of British Columbia**)
- Self-driving labs for CO₂ membrane electrode assemblies (**University of British Columbia**)
- Specialty chemical electrosynthesis from CO₂ (**University of Toronto**)



CO₂
Conversion

Cross Platform

- Technoeconomic assessments and life cycle analysis of CO₂ conversion (**University of Calgary, University of Toronto, University of Alberta, University of Michigan, NETL**)

Photocatalytic

- Solar dry reforming of CO₂ into fuels (**Solistra**)
- Solar fuels for carbon neutral transport (**University of Waterloo**)
- Scalable plasmonic catalysts for CO₂ conversion (**University of Ottawa**)

Thermocatalytic

- Direct conversion of CO₂ rich flue gas to syngas (**University of Sherbrooke**)
- CO₂ to jet fuel technology platform (**Ecole Polytechnique Montreal**)

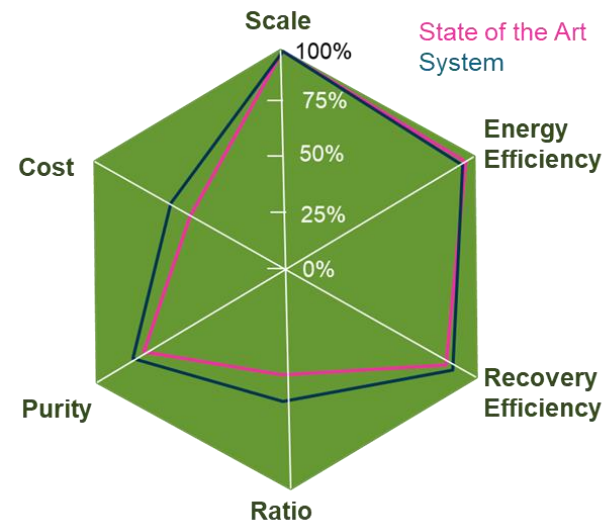
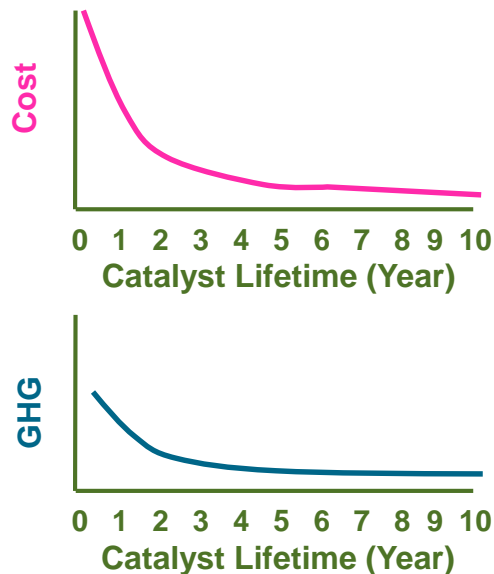
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Contributions
Awarded

Technoeconomic and Lifecycle Assessments for CCUS



Ryan Baker, Miyuru Kannangara, Jianjun Yang and Cyrille Deces-Petit, Mauro Dalcin, Farid Bensebaa
Work in progress

THANK YOU

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