

Environment and Natural Resources Trust Fund

2025 Request for Proposal

General Information

Proposal ID: 2025-257

Proposal Title: Facilitated Transport Hybrid Membranes for CO2 Separation

Project Manager Information

Name: Jun Li Organization: U of MN - College of Science and Engineering Office Telephone: (612) 626-0153

Email: junli1@umn.edu

Project Basic Information

Project Summary: To capture CO2, we will develop advanced polymeric membranes infused with metal-organic framework nanoparticles. These membranes facilitate the passage and collection of CO2 while blocking the permeation of other gases.

ENRTF Funds Requested: \$1,150,000

Proposed Project Completion: June 30, 2028

LCCMR Funding Category: Air Quality, Climate Change, and Renewable Energy (E)

Project Location

What is the best scale for describing where your work will take place? Statewide

What is the best scale to describe the area impacted by your work? Statewide

When will the work impact occur?

During the Project and In the Future

Narrative

Describe the opportunity or problem your proposal seeks to address. Include any relevant background information.

CO2 emissions have a huge impact on the global carbon cycle. It is well-documented that CO2 is a greenhouse gas and one of the main contributors to global warming. Also, the accumulation of CO2 in the atmosphere results in a reduction in the pH of the upper ocean. Reducing CO2 emissions remains a major challenge to mankind. A solution that sequesters atmospheric CO2 will bring enormous environmental benefits. Various CO2 capture technologies include absorption, adsorption, membrane, biological capture, and cryogenic capture. Compared to other separation methods, membrane separation is generally more energy efficient and environmentally benign, thus has been intensively studied for CO2 capture.

What is your proposed solution to the problem or opportunity discussed above? Introduce us to the work you are seeking funding to do. You will be asked to expand on this proposed solution in Activities & Milestones.

We will design and develop highly permeable and highly selective membranes, termed facilitated transport hybrid membranes (FTHMs), by integrating functionalized metal-organic framework (MOF) particles into a polymer matrix. These tailored membranes aim to facilitate the transport of CO2 molecules while effectively blocking other gases typically found in emission sources. FTHM would enable the capture and collection of CO2 for subsequent utilization.

By harnessing the unique properties of functionalized MOFs, our membranes are expected to outperform conventional polymeric and hybrid membranes (HMs), which rely on inorganic nanoparticles. This superiority stems from (i) the chemical affinity and compatibility of MOFs with the polymer, and (ii) the incorporation of specific functional groups onto the MOFs to enable reversible reactions with CO2, thereby boosting the efficiency of CO2 transport across the membrane.

Our specific objectives are:

- 1. Develop MOFs for optimal facilitated transport and incorporation into FTHM.
- 2. Design a robust fabrication method that can uniformly distribute the MOF particles within the polymer matrix.
- 3. Deliver an FTHM and compare its CO2 permeability and selectivity with that of state-of-the-art HMs for CO2 capture.

4. Deliver a membrane contactor for CO2 separation and compare its performance with that of state-of-the-art membrane contactors.

What are the specific project outcomes as they relate to the public purpose of protection, conservation, preservation, and enhancement of the state's natural resources?

The proposed membranes are highly relevant to CO2 emission in Minnesota, specifically to localized emission sources in industrial facilities that continue to use oil and natural gas to heat and operate. Emissions from these sources have risen 14% between 2005 and 2020 (Greenhouse gas emission in Minnesota 2005-2020, Report to the Legislature January 2023). The target membranes are intended to improve the performance of equipment that can reduce such emissions directly at their source.

Activities and Milestones

Activity 1: High performance molecular dynamics computational simulation studies of gas separation in a MOF-based FTHM (Dumitrică)

Activity Budget: \$229,868

Activity Description:

These atomic level simulations are expected to fill key knowledge gaps in our understanding of the factors that limit and enhance the separation performances of FTHMs. Specifically, concentration gradient-driven non-equilibrium molecular dynamics simulations will quantify and characterize the gas transport dynamics at the polymer/MOF interface. We hypothesize that processes occurring at this interface exerts a pivotal influence on the performance of the FTHM. We will construct atomistic models of the polymer/MOF interface and utilize them to investigate the surface compatibility between the polymer and the MOF, both with and without functional groups. Our aim is to capture in the simulations the potentially detrimental effects of interfacial defects, like nonselective voids and the benefits of functional groups added to MOF, and ultimately to establish a connection between simulated compatibility and the real-world performance of FTHM. In addition to delivering an unprecedented microscopic picture of transport and formulating predictions (including idealized predictions) of the separation performance based on the individual constituents of a FTHM, the constituent screening afforded by these simulations (performed ahead of experimentation) will play a guiding role in the FTHM materials selection and interface design through MOF functionalization for the next-generation HMs for CO2 separation.

Activity Milestones:

Description	Approximate Completion Date
1.1 Simulation of membranes of polymer/UiO-66 MOF (nonfunctionalized) with and without interfacial voids	September 30, 2025
1.2 Computational optimization of membranes of polymer/UiO-66 (functionalized) with and without interfacial voids	December 31, 2025
1.3 Simulation of membranes of polymer/other MOFs (functionalized) with and without interfacial voids	September 30, 2026
1.4 Computational optimization of membranes of polymer/the most promising MOF (functionalized)	September 30, 2027
1.5 High throughput simulations for FHTM materials selection of next-gen membranes	March 31, 2028

Activity 2: Fabrication and characterization of MOF-based FTHMs (Stein, Li)

Activity Budget: \$499,803

Activity Description:

In Budget Period 1, we plan to optimize the design of the UiO-66-based FTHM based on a previous 3M-funded seed project and the computational guidance in Activity 1. Then, we will fabricate the optimized UiO-66-based FTHM. Following that, we will characterize the FTHM, focusing on the dispersion of the functionalized UiO-66 in the polymer matrix and the durability of the FTHM.

In Budget Period 2, we plan to fabricate FTHMs of polymer/other functionalized MOFs based on information from Activity 1. Specifically, we are interested in using 2D MOFs. Besides having reversible reactions with CO2, the 2D MOFs could also possibly act as diffusion barriers for other gases, assuming only weak interactions with those gases, to achieve high selectivities. We will use characterization to verify dramatically improved dispersion of the functionalized MOF throughout the membrane and extraordinary durability for the optimized FTHM. We anticipate seeing improvements in the facilitate transport mechanism for it, too, which will be reflected by a higher CO2 sorption coefficient of the FTHM.

In Budget Period 3, we plan to scale up the optimized MOF-based FTHM, in order to make our FTHM more ready technically and practically.

Activity Milestones:

Description	Approximate Completion Date
2.2 Fabrication of optimized FTHM of polymer/UiO-66 (functionalized) based on 1.2	March 31, 2026
2.3 Characterization of FTHM from 2.2. Verify dispersion of functionalized UiO-66 and durability	June 30, 2026
2.1 Synthesis and characterization of MOF particles	December 31, 2026
2.4 Fabricate FTHMs of polymer/other MOFs based on 1.4 and 1.5	June 30, 2027
2.5 Characterization of FTHMs from 2.4. Verify dispersion of functionalized MOFs and durability	September 30, 2027
2.6 Scale-up of optimized MOF-based FTHM	December 31, 2027

Activity 3: Testing of CO2 permeation and sorption performance of MOF-based FTHMs (Li)

Activity Budget: \$139,183

Activity Description:

In Budget Period 1, we will build a high-fidelity gas sorption test facility that can accurately quantify the facilitated transport performance for membranes. We will use an existing gas permeation test facility from a previous 3M-funded seed project to measure CO2 permeation performance for our membranes.

We will measure the CO2 permeability and selectivity of the FTHM developed in Activity 2.2 using the gas permeation test facility. We will verify that there is improved performance compared to previously developed UiO-66-based FTHMs from the previous 3M-funded seed project.

We will measure the CO2 solubility of the FTHM developed in Activity 2.2 using the gas sorption test facility. The CO2 sorption coefficient will be derived based on the results. We will use that to verify the improvements in the facilitate transport mechanism and the advantages of our design.

In Budget Period 2, we plan to perform the same tests described above to the FTHMs developed in Activity 2.4 (using other MOFs), which are supposed to have even higher performance than those from Activity 2.2. We will verify that the CO2 permeability and selectivity of optimized one are both dramatically higher than the state-of-the-art HMs.

Activity Milestones:

Description	Approximate Completion Date
3.1 Build-up of gas sorption test facility for membranes	March 31, 2026
3.2 Testing of the FTHM developed in Activity 2.2	June 30, 2026
3.3 Testing of FTHMs developed in Activity 2.4	June 30, 2027

Activity 4: Testing of CO2 separation performance of membrane contactors using MOF-based FTHMs (Li)

Activity Budget: \$181,146

Activity Description:

To make our technology more ready for applications, starting from Budge Period 2, we will build a test facility for membrane contactors for CO2 separation. We will also design and fabricate novel contactors for CO2 separation using the scaled-up, optimized MOF-based FTHM from Activity 2.6. Finally, we will test these membrane contactors.

Our design target is the effectiveness of our best membrane contactor for CO2 separation is much higher than that of state-of-the-art membrane contactors.

Activity Milestones:

Description	Approximate Completion Date
4.1 Build-up of the test facility for membrane contactors for CO2 separation	September 30, 2027
4.2 Novel design of membrane contactors for CO2 separation	September 30, 2027
4.3 Fabrication of CO2 separation membrane contactors using FTHMs developed in Activity 2.6	March 31, 2028
4.4 Testing of membrane contactors developed in Activity 4.3	June 30, 2028

Activity 5: Field testing of CO2 separation membrane contactors using MOF-based FTHMs (Li, contractor)

Activity Budget: \$100,000

Activity Description:

This activity aims to examine the performance of our CO2 separation membrane contactor in the field. We plan to hire a professional CO2 emission evaluation organization as a contractor to finish this activity. Near the end of Budget Period 2, we will start to identify a facility to test our membrane contactor. Our focus will be industrial CO2 emission facilities. We will fabricate a membrane contactor using FTHMs developed in 2.6 and provide it to the CO2 emission evaluation organization to test.

Activity Milestones:

Description	Approximate Completion Date
5.1 Identify an industrial CO2 emission facility for field testing	December 31, 2027
5.2 Fabrication of a CO2 separation membrane contactor using FTHMs developed in 2.6	March 31, 2028
5.3 Install the CO2 separation membrane contactor and testing instrumentation onsite. Test the	June 30, 2028
contactor	

Project Partners and Collaborators

Name	Organization	Role	Receiving
	-		Funas
Andreas Stein	U of MN -	Professor Stein's expertise includes zeolite and MOF syntheses, zeolite	Yes
	College of	membranes, and functionalization of delaminated clay or graphene oxide	
	Science and	materials for polymer nanocomposite fabrication with improved structural and	
	Engineering	barrier properties. He will lead the synthesis, functionalization, and	
		characterization of the MOF particles, as well as the characterization of FTHMs.	
Traian	U of MN -	Professor Dumitrică's expertise includes molecular dynamics computations for	Yes
Dumitricã	College of	describing the fundamental mechanical deformations of nano-materials,	
	Science and	determining optimal equilibrium nano-structures, and investigating the transport	
	Engineering	properties of nano-system. He will lead the molecular dynamics computational	
		effort to provide design guidance for the component materials of our FTHMs.	
Michael Kesti	3M Company	3M will work with us as an industrial partner. They will provide perspectives from	No
		the industry. They are also considering providing us with their proprietary MOFs.	
		They will look into opportunities to commercialize our research outcomes (i.e.	
		contactor and membranes) after the project provided the results are promising.	

Long-Term Implementation and Funding

Describe how the results will be implemented and how any ongoing effort will be funded. If not already addressed as part of the project, how will findings, results, and products developed be implemented after project completion? If additional work is needed, how will this work be funded?

The findings and results will be disseminated to federal and state agencies, industries, and other interested parties, through open-access publications and conference presentations.

3M, as our industrial partner, will scale up our technology and commercialize our technology provided that the results for membranes and contactors in this project are promising.

If new avenues for research emerge from this combined experimental-computational research effort, we will apply for funding from federal sources such as the U.S. Environmental Protection Agency (EPA), the National Science Foundation (NSF), the Department of Energy (DOE), etc.

Project Manager and Organization Qualifications

Project Manager Name: Jun Li

Job Title: Richard and Barbara Nelson Assistant Professor

Provide description of the project manager's qualifications to manage the proposed project.

Prof. Jun Li will serve as the project manager. Prof. Li's research to-date has involved polymer and surface sciences for anti-icing and antifouling applications, liquid-vapor phase separation and distribution in microchannel heat exchangers, and in-tube phase-change heat transfer. Prof. Li's postdoctoral research focused on surfaces and coatings for anti-icing and antifouling applications. His Ph.D. research mainly focused on heat transfer, multiphase flow, and thermal systems. At UMN, Prof. Li's research focuses on polymer science. He designs synthetic materials for carbon capture and designs synthetic coatings to control the accretion of various matters and applies them to thermal fluid components and systems, with the end goal of decarbonization for the energy sector of the society.

In this project, Prof. Li will handle the overall project management and planning. On the fabrication side of the project, he will lead the synthesis of the polymer matrix for the FTHMs, the fabrication of the FTHMs, and the scale-up of the FTHMs. On the testing side of the project, he will lead the CO2 permeation and sorption tests to verify the performance of the membranes. He will also design and fabricate novel membrane contactors using the optimized FTHMs, and then

verify the improved performance of the membrane contactors compared to the state-of-the-art.

Currently, Prof. Li is working as the Principle Investigator (PI) for a 3M-funded seed project with Prof. Andreas Stein. This experience will provide a seamless transition for Prof. Li to continuously work with Prof. Stein for the LCCMR project, with 3M being the industrial partner. Besides that, Prof. Li has submitted a large-scale (~\$2M) research proposal (currently under review) to the U.S. Department of Energy as the PI. In that proposal, he coordinated a team of UMN, a Fortune 500 company that delivers HVAC technologies, and a technical consulting firm.

Organization: U of MN - College of Science and Engineering

Organization Description:

The University of Minnesota is the main research and graduate teaching institution in the state of Minnesota. The Department of Mechanical Engineering is building on the past, responding to the present, and leading the way to the future by driving innovative research with significant real-world impact through our five impact areas: Environment & Sustainability, Energy Transition, Human Health, Next-Gen Manufacturing, and Robotics & Mobility. For Environment & Sustainability, from the atmosphere to ground water and everything in between, mechanical engineering is essential in the advancement of environment and sustainability studies. Researchers in the Department of Mechanical Engineering work on air and water pollution, seawater desalination, engine efficiency, alternative fuels, biodegradables, and more to combat climate change and work toward a greener future.

Budget Summary

Category / Name	Subcategory or Type	Description	Purpose	Gen. Ineli gible	% Bene fits	# FTE	Class ified Staff?	\$ Amount
Personnel								
Jun Li		PI			27.06%	0.27		\$37,818
Traian Dumitrica		Co-PI			27.06%	0.27		\$46,713
Andreas Stein		Co-PI			27.06%	0.27		\$58,747
ME Research Assistants		Research Assistants			43.64%	4.5		\$549,465
Chem Research Assistants		Research Assistants			51.32%	1.5		\$179,294
							Sub Total	\$872,037
Contracts and Services								
TBD	Professional or Technical Service Contract	We plan to hire a professional CO2 emission evaluation organization to perform field tests for our CO2 separation membrane contactor. We will identify a facility to test our membrane contactor. The professional service will install the membrane contactor and testing instrumentation onsite and evaluate our membrane contactor.				0		\$100,000
							Sub Total	\$100,000
Equipment, Tools, and Supplies								
	Equipment	Maxwell Robotics UB-C-1106-004 thermoelectric heater/chiller module. Quantity: 1	Build-up of gas sorption test facility for membranes					\$4,500
	Equipment	Maxwell Robotics UB-C-1106-003 Dual-pressure range pressurization system. Quantity: 1	Build-up of gas sorption test facility for membranes					\$4,500
	Equipment	Maxwell Robotics UB-C-1106-002 gas injection valve. Quantity: 5	Build-up of gas sorption test facility for membranes					\$7,495
	Equipment	Swagelok Diaphragm Valves 6LVV-DPHFR4-P-C. Quantity: 4	Build-up of gas sorption test facility for membranes					\$2,000
	Equipment	Thermo-Fisher temperature controller. Quantity: 1	Build-up of gas sorption test facility for membranes					\$1,505

Equipment	Thermo-Fisher SC-150 temperature controller. Quantity: 2	Build-up of the test facility for membrane contactors for CO2	\$5,660
	2	separation	
Equipment	MKS Baratron 622D11TBE capacitance manometer. Quantity: 4	Build-up of the test facility for membrane contactors for CO2	\$4,200
 Equipment	Feed solution pump. Quantity: 1	Build-up of the test facility for membrane contactors for CO2	\$2,500
 Equipment	Absorption solution pump. Quantity: 1	Build-up of the test facility for membrane contactors for CO2 separation	\$2,500
Equipment	ATO variable frequency drive (VFD) + Dayton general purpose motor. Quantity: 2	Build-up of the test facility for membrane contactors for CO2 separation	\$4,000
Equipment	Customized stainless steel feed tank. Quantity: 1	Build-up of the test facility for membrane contactors for CO2 separation	\$4,000
Equipment	Customized absorption tank. Quantity: 1	Build-up of the test facility for membrane contactors for CO2 separation	\$4,000
Equipment	Customized gas mixer. Quantity: 1	Build-up of the test facility for membrane contactors for CO2 separation	\$900
Equipment	Customized gas-liquid separator. Quantity: 1	Build-up of the test facility for membrane contactors for CO2 separation	\$950
Equipment	Danfoss condenser. Quantity: 2	Build-up of the test facility for membrane contactors for CO2 separation	\$1,600
Equipment	Fisherbrand Maxima rotary vane vacuum pump. Quantity: 1	Build-up of the test facility for membrane contactors for CO2 separation	\$1,930
Equipment	OMEGA HX85BA hygrometer. Quantity: 2	Build-up of the test facility for membrane contactors for CO2 separation	\$1,900
Equipment	Swagelok diaphragm valves. Quantity: 5	Build-up of the test facility for membrane contactors for CO2 separation	\$1,930
Equipment	Membrane contactors for CO2 separation. Quantity: 5	Fabrication of CO2 separation contactors using the FTHMs for in-lab tests and field tests	\$6,000

	Equipment	Omega absolute pressure transducer. Quantity: 1	Build-up of the test facility for membrane contactors for CO2 senaration			\$893
	Tools and Supplies	Chemicals and general laboratory supplies and consumables. Quantity: N/A	Synthesis of MOFs and polymers needed for FTHM fabrication			\$30,000
					Sub Total	\$92,963
Capital Expenditures						
		Maxwell Robotics UB-201-X control system. Quantity: 1.	Build-up of gas sorption test facility for membranes	х		\$15,000
		ThermoFisher TRACE gas chromatography (GC) analyzer. Quantity: 1	Build-up of the test facility for membrane contactors for CO2 separation	Х		\$15,000
		Micro Motion ELITE mass flow meter and transmitter. Quantity: 1	Build-up of the test facility for membrane contactors for CO2 separation	Х		\$15,000
					Sub Total	\$45,000
Acquisitions and Stewardship						
					Sub Total	-
Travel In Minnesota						
					Sub Total	-
Travel Outside Minnesota						
					Sub Total	-
Printing and Publication						
	Publication	Open access publication fee. Quantity: N/A	Disseminating the work and make our results publicly available.			\$4,000
					Sub Total	\$4,000
Other Expenses						

	Scientific Services. Quantity: N/A	Characterization of materials synthesized in this project (MOFs and membranes) at the UMN Characterization Facility and UMN Polymer Characterization and Processing Facility.			\$36,000
				Sub	\$36,000
				Total	
				Grand	\$1,150,000
				Total	

Classified Staff or Generally Ineligible Expenses

Category/Name	Subcategory or Type	Description	Justification Ineligible Expense or Classified Staff Request
Capital Expenditures		Maxwell Robotics UB-201-X control system. Quantity: 1.	The Maxwell Robotics UB-201-X control system, as the system controller, is an indispensable for the gas sorption test facility. The UB-201-X is an embedded Linux computer system with a touch screen interface. It coordinates all system functions, such as gas flow sequencing, pressure control, temperature control, etc. Additional Explanation : The Maxwell Robotics UB-201-X control system is an indispensable part of the gas sorption test facility. It will be used as long as the gas sorption test facility is used for testing CO2 sorption.
Capital Expenditures		ThermoFisher TRACE gas chromatography (GC) analyzer. Quantity: 1	Gas chromatography (GC) analyzer is used to separate and quantify each compound in a gas mixture. We will use it to analyze the downstream flow after the membrane contactor. It is a necessary piece of instrument for the test facility. Additional Explanation : The GC analyzer will stay with the test facility for membrane contactors. The test facility will be used continuously for measuring the performance of various membrane contactors for CO2 separation.
Capital Expenditures		Micro Motion ELITE mass flow meter and transmitter. Quantity: 1	The mass flow meter is necessary for measuring the mass flow rate of separated CO2 flow in the test facility for membrane contactors for CO2 separation. We will need this quantity to derive the effectiveness of CO2 separation by the membrane contactor. Additional Explanation : The mass flow meter is an indispensable part of the test facility for membrane contactors for CO2 separation. It will be continuously used for the same kind of research.

Non ENRTF Funds

Category	Specific Source	Use	Status	Amount
State				
			State Sub	-
			Total	
Non-State				
In-Kind	unrecovered F&A calculated at 55% MTDC	Support of ME facilities where research will be conducted.	Secured	\$488,888
			Non State	\$488,888
			Sub Total	
			Funds	\$488,888
			Total	

Total Project Cost: \$1,638,888

This amount accurately reflects total project cost?

Yes

Attachments

Required Attachments

Visual Component File: <u>8672ac73-37a.pdf</u>

Alternate Text for Visual Component

Summary chart to demonstrate the project plan...

Supplemental Attachments

Capital Project Questionnaire, Budget Supplements, Support Letter, Photos, Media, Other

Title	File
3M Letter of Support	74ce1e2d-fde.pdf
University of Minnesota Authorization Letter	03e435fd-20a.pdf

Administrative Use

Does your project include restoration or acquisition of land rights?

No

Does your project have potential for royalties, copyrights, patents, sale of products and assets, or revenue generation?

Yes

Do you understand and acknowledge IP and revenue-return and sharing requirements in 116P.10?

Yes

- Do you wish to request reinvestment of any revenues into your project instead of returning revenue to the ENRTF? No
- Does your project include original, hypothesis-driven research?

Yes

Does the organization have a fiscal agent for this project?

No

Does your project include the pre-design, design, construction, or renovation of a building, trail, campground, or other fixed capital asset costing \$10,000 or more or large-scale stream or wetland restoration?

No

Do you propose using an appropriation from the Environment and Natural Resources Trust Fund to conduct a project that provides children's services (as defined in Minnesota Statutes section 299C.61 Subd.7 as "the provision of care, treatment, education, training, instruction, or recreation to children")?

No

Provide the name(s) and organization(s) of additional individuals assisting in the completion of this proposal:

N/A