Environment and Natural Resources Trust Fund

2022 Request for Proposal

General Information

Proposal ID: 2022-180

Proposal Title: Green Solar Cells from a Minnesota Natural Resource

Project Manager Information

Name: Chris Leighton

Organization: U of MN - College of Science and Engineering

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Project Basic Information

Project Summary: Recent U of M breakthroughs will be built upon to realize the first truly environmentally friendly solar cells, simultaneously unlocking exciting new renewable energy opportunities for the MN Iron Range.

Funds Requested: $756,000

Proposed Project Completion: June 30 2025

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.

It is now widely accepted that climate change is underway, that it results from human activity, and that it will soon induce global changes of enormous concern. The development of renewable energy sources to mitigate climate change thus may be the defining challenge of our time. Due to the abundance of sunlight, solar power will undoubtedly form part of the solution. In the context of the environment, however, it is imperative that materials used in solar cells (photovoltaics) be fundamentally "green", i.e., non-toxic, earth-abundant, low-carbon-cost, etc. Strikingly, this is not true of current photovoltaics. Silicon, for example, requires so much electricity for its production that the time to "net neutral carbon" is years. Competitors like cadmium telluride and copper indium gallium selenide are yet worse, being based on toxic (e.g., cadmium), rare (e.g., tellurium), or sensitive elements (e.g., indium), for which reliance on foreign resources is up to 100%. Materials called perovskites are rapidly emerging as alternatives, but are typically based on highly toxic lead. We thus lie on the verge of solving one environmental problem only to create numerous others. Developing fundamentally "green" solar cell materials is thus a grand scientific challenge, directly addressed here.

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

We propose an innovative solution, not only developing a fundamentally "green" solar cell material, but doing so with MN natural resources. This emerges from a decade-long effort by Leighton and collaborators at the U, focusing on the extraordinary material iron disulfide, otherwise known as pyrite or fool's gold (Figure 1). This photovoltaic is not only based on low-toxicity, earth-abundant elements but is also estimated to be 100 times cheaper than its nearest competitor and 10,000 times cheaper than silicon (Figure 1). This is due to the negligible cost of sulfur (a globally-stockpiled waste product (Figure 2)) and the massive abundance of iron. The semiconducting properties of pyrite, essential for photovoltaics, are also near-ideal. Despite this promise, the efficiency of pyrite solar cells has barely exceeded 3%, ten times below its potential. Motivated by this, Leighton and collaborators invested a decade of research into understanding and eliminating roadblocks to pyrite photovoltaics. This has been highly productive, culminating in 2020 in the identification of the origin of poor solar cell efficiency, and the first viable route to circumvent it (using "homojunction" solar cells). Here, we propose to translate these breakthroughs into real applications, realizing the first efficient pyrite solar cells.

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?

Vitally, our proposed work could not only realize the first truly "green" solar cell technology, but could do so with MN natural resources. Specifically, pyrite solar cells would need to be based on precisely-engineered synthetic pyrite formed from sulfur and iron. Efficient pyrite solar cells thus create the possibility of using MN Iron Range resources (Figure 2) in a fundamentally renewable energy technology, in stark contrast to their current use in carbon-costly steel production. To this end, we will thus also make a materials/geology/natural-resource-science-based evaluation of the feasibility of using Iron Range resources to manufacture this "green" photovoltaic.

Activities and Milestones

Activity 1: 1. Completing the understanding of pyrite electronic and opto-electronic properties

Activity Budget: $226,800

Activity Description:

The prior work of Leighton essentially identified three possible origins of poor efficiency in pyrite solar cells: (i) unwanted secondary phases (e.g., FeS in FeS2); (ii) difficulties with “doping” (the process used to control properties of photovoltaics); and (iii) irregularities with pyrite surfaces. Possibility (i) was comprehensively eliminated. Significant advances were then made with (ii), resolving a problem known as the “pyrite doping puzzle”, and proving that typical pyrite doping occurs due to defects called sulfur vacancies (missing sulfur atoms). Control was then demonstrated, leading to tunable “n-type” doping, i.e., controlled concentrations of electrons. The most significant advance, however, came in (iii), through the discovery that anomalous electronic properties of pyrite surfaces are the specific origin of poor solar cell performance. Vitally, these advances point to the first viable route to circumvent the problems with existing pyrite solar cells. This route is a “homojunction” cell, essentially a junction between two differently-doped pyrite regions (called "n-type" and "p-type"). Activity 1 will thus address the final barriers to the first efficient pyrite homojunction solar cells: improved control of n-type doping, development of an effective p-type dopant, and improved understanding of pyrite optoelectronics, i.e., its conversion of light to electricity.

Activity Milestones:

Description	Completion Date
A. Development of phosphorous as a p-type dopant in pyrite	December 31 2022
B. Exploration of ultralow-sulfur-vacancy-density pyrite	June 30 2023
C. Photophysics studies of n- and p-type pyrite	June 30 2023
D. Control of the S vacancy energy level in pyrite	December 31 2023
E. Photophysics studies of pyrite p-n homojunctions	December 31 2023

Activity 2: 2. Developing efficient pyrite homojunction solar cells

Activity Budget: $378,000

Activity Description:

The goal of Activity 2 is to build on recent breakthroughs in the understanding of pyrite, in addition to knowledge from Activity 1, to drive this technology from science to applications. The essential concept is that prior pyrite solar cells were based on “heterojunctions” i.e., interfaces between other materials and pyrite surfaces. Armed with the new understanding that these surfaces behave anomalously, limiting performance, pyrite homojunction cells become the central goal. Our first goal in Activity 2 will therefore be to develop strategies to eliminate parasitic surface effects in homojunctions. Treatments using ion beams will be tested, eliminating surface conduction, and enabling us to properly test homojunctions. Following this, we will explore two routes to p-n homojunction solar cells: naturally-formed internal p-n junctions due to p-type surfaces on n-type crystals, and artificially-fabricated p-n junctions using approaches known as “contact doping” and “ion implantation”. We will then perform extensive electrical characterization, culminating in solar cell testing, i.e., under solar illumination. Finally, to exploit pyrite's extraordinarily high light absorption, pyrite solar cells should ultimately be based on very thin films of the material (to minimize materials costs); we will thus also explore translation of this research towards thin film devices.

Activity Milestones:

Description	Completion Date
A. Development and testing of device isolation strategies (controlling surface conduction)	June 30 2023
B. Electrical testing of p-n homojunctions	June 30 2024

C. Solar cell testing of p-n homojunctions	June 30 2025
D. Translation from single-crystal to thin-film devices	June 30 2025

Activity 3: 3. Assessing the feasibility of MN Iron Range iron for the manufacture of pyrite-based "green" solar cells.

Activity Budget: $151,200

Activity Description:
An important feature of pyrite solar cells is that they would be fabricated from earth-abundant sulfur and iron (mineral pyrite cannot be used due to uncontrolled electronic properties), thus creating a potential renewable energy application for a key MN resource. Activity 3 will combine the Twin Cities faculty expertise (materials science, electrical engineering, chemistry), with the expertise of Hudak (geology, natural resources), to make the first assessment of the feasibility of using Iron Range resources for synthesis of this photovoltaic. Iron Range hematite samples from both the taconite process and an emerging ilmenite process will be converted to iron, then used to synthesize pyrite crystals and films. We will then conduct extensive testing, assessing purity, structural quality, electronic/optical properties, etc. Direct conversion of hematite to pyrite will also be explored, potentially streamlining the process. Importantly, all of these approaches should induce substantial purification during synthesis, as required for photovoltaics. Finally, Hudak will also perform an analysis of the economics of utilizing Iron Range resources for photovoltaic pyrite synthesis. Critical factors such as the availability of appropriately-pure MN iron, production costs, and environmental impacts will be considered, providing the first assessment of the feasibility of this emerging renewable energy application.

Activity Milestones:

Description	Completion Date
A. Conversion of Iron Range hematite to iron	December 31 2022
B. Fabrication and testing of pyrite crystals and thin films from Iron Range iron	June 30 2024
C. Direct conversion of Iron Range hematite to pyrite	December 31 2024
D. Geologic/materials/natural-resource-science-based assessment of feasibility	June 30 2025

Project Partners and Collaborators

Name	Organization	Role	Receiving Funds
Prof. Renee Frontiera	Department of Chemistry, University of Minnesota (Twin Cities)	Prof. Frontiera, collaborating with Leighton, will lead aspects of the proposed work related to pyrite photophysics/opto-electronics, i.e., how pyrite absorbs light, creates carriers of electricity (electrons), and how these carriers move. She is a renowned expert on the study of these processes at high time and spatial resolution.	Yes
Dr. George Hudak	Natural Resources Research Institute, University of Minnesota (Duluth)	Dr. Hudak, collaborating with Leighton, will lead aspects of the proposed work related to assessing the geologic/natural resource science feasibility of using MN Iron Range iron to manufacture pyrite solar cells. He is a renowned expert on economic geology, actively working on issues related to the MN Iron Range.	Yes
Prof. Steve Koester	Department of Electrical and Computer Engineering, University of Minnesota (Twin Cities)	Prof. Koester, collaborating with Leighton, will lead aspects of the proposed work related to solar cell device design, fabrication, and testing. He is a renowned expert on semiconductor opto-electronic devices with expertise both in academia and industry (including 14 years at IBM).	Yes

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 be funded?

This proposed work builds on substantial prior research, funded primarily by federal and state sources. We will now leverage this to translate these scientific breakthroughs towards a real technology, via the demonstration of the first efficient pyrite-based solar cells. Such a demonstration is highly likely to enable subsequent fundraising from more applied/technological programs (both government (e.g., Department of Energy) and industrial), to move beyond demonstration solar cells. In essence, what is needed now is the support of a program willing to back an emerging technology with extraordinary renewable energy potential, specifically tied to Minnesota natural resources.

Project Manager and Organization Qualifications

Project Manager Name: Chris Leighton

Job Title: Distinguished McKnight University Professor

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

Chris Leighton is a Distinguished McKnight University Professor and Distinguished University Teaching Professor of Chemical Engineering and Materials Science at the University of Minnesota (U of M). Following B.Sc. and Ph.D. degrees in Physics at the University of Durham (1994, 1998), and post-doctoral research at the University of California San Diego, he joined the U in 2001. His research focuses on materials for electronic devices, including low-cost, non-toxic, earth-abundant photovoltaics, i.e., materials for environmentally-friendly ("green") solar cells. He has authored 220 scientific publications, which have been cited 12,000 times. He is a Fellow of various scientific societies (e.g., the American Physical Society and Institute of Electrical and Electronics Engineers), and has been recognized via a Cozzarelli Prize from the National Academy of Sciences, and the U of M's McKnight Presidential Fellowship, Taylor Distinguished Research Award, and Distinguished McKnight University Professorship.

Most significantly for this proposal, Leighton has dedicated over a decade of research effort to exploring and developing materials for "green" solar cells. This has narrowed in on a remarkable material - iron disulfide, otherwise known as pyrite or fool's gold - as a uniquely low-cost, earth-abundant, non-toxic photovoltaic, also identifying the first viable route to efficient solar cells based on this material. The goal of this proposal is to translate these scientific breakthroughs to real applications, demonstrating the first efficient pyrite-based solar cells. Critically, such solar cells must be synthesized from sulfur and iron, the latter being a singularly important MN resource. Success in this proposed work would thus not only realize the first truly environmentally-friendly solar cells, but also create extraordinary renewable energy opportunities for the MN Iron Range. In terms of project management, Leighton has 20 years of experience overseeing research and development projects, funded by government and industrial sources.

Organization: U of MN - College of Science and Engineering

Organization Description:
The proposed research and development will be performed by Leighton and a team of collaborators (Prof. Renee Frontiera, Prof. Steve Koester, and Dr. George Hudak), on the U of M's Twin Cities and Duluth campuses. Leighton, Frontiera, and Koester bring expertise from the Departments of Chemical Engineering and Materials Science, Chemistry, and Electrical and Computer Engineering, while Hudak brings expertise from the Duluth Natural Resources Research Institute. Together, these U of M faculty provide all the required expertise and capabilities in materials science, electrical engineering, physics, chemistry, geology, and natural resource science, not only to develop efficient pyrite-based solar cells, but also to assess the feasibility of utilizing MN Iron Range resources in this "green" energy technology. The labs of these faculty, complemented with various shared facilities readily available at the U, provide all technical capabilities required for this work. Moreover, and as emphasized throughout this proposal, it is U of M research that led to the remarkable scientific breakthroughs that bring us to the verge of utilizing this uniquely attractive low-cost, non-toxic, earth-abundant solar cell material. The U of M is thus uniquely positioned to perform this research, additionally being situated in the nation's largest iron-producing state.

Budget Summary

Category / Name	Subcategory or Type	Description	Purpose	Gen. Ineligible	% Benefits	# FTE	Classified Staff?	$ Amount
Personnel								
Principal Investigator		Chris Leighton, principal Investigator			26.7%	0.12		$37,128
Co-Investigator		Renee Frontiera, co-Investigator			26.7%	0.12		$25,964
Co-Investigator		Steve Koester, co-Investigator			26.7%	0.12		$39,292
Postdoctoral Research Associate		Postdoctoral Research Associate, Chemical Engineering and Materials Science			20.25%	3		$189,536
Graduate Research Assistant		Graduate Research Assistant, Chemistry			22.74%	1.5		$106,098
Graduate Research Assistant		Graduate Research Assistant, Electrical and Computer Engineering			43.7%	1.5		$151,764
Co-Investigator		George Hudak, co-Investigator			26.7%	0.3		$55,415
							Sub Total	**$605,197**
Contracts and Services								
University of Minnesota shared facility usage (Characterization Facility and Minnesota Nano Center)	Internal services or fees (uncommon)	These two University of Minnesota shared facilities (the Characterization Facility and Minnesota Nano Center) are essential to perform this research. They house many of the laboratory instruments required for the work, which are accessed on an hourly-charge basis by student and post-doctoral researchers.				-		$67,500
							Sub Total	**$67,500**
Equipment, Tools, and Supplies								
	Tools and Supplies	Lab materials and supplies	Purchase of standard lab materials and supplies (chemicals, gases, glassware, etc.)					$67,500

							Sub Total	**$67,500**
Capital Expenditures								
							Sub Total	**-**
Acquisitions and Stewardship								
							Sub Total	**-**
Travel In Minnesota								
							Sub Total	**-**
Travel Outside Minnesota								
	Conference Registration Miles/ Meals/ Lodging	Approximately 1 trip per year for each of the 4 research groups involved in the work. This will be typically be national air travel, lodging, meals, registration, etc.	Presentation of latest research results at national conferences, meetings and workshops.					$15,803
							Sub Total	**$15,803**
Printing and Publication								
	Publication	Publication of scientific/engineering papers resulting from the research. This will be done in society-based journals that have no page charges. Thus there are no costs in this category.	Publication of the key research results will be a vital product of the proposed work.					-
							Sub Total	**-**
Other Expenses								
							Sub Total	**-**
							Grand Total	**$756,000**

Classified Staff or Generally Ineligible Expenses

Category/Name	Subcategory or Type	Description	Justification Ineligible Expense or Classified Staff Request

Non ENRTF Funds

Category	Specific Source	Use	Status	Amount
State				
			State Sub Total	**-**
Non-State				
			Non State Sub Total	**-**
			Funds Total	**-**

Attachments

Required Attachments

Optional Attachments

Support Letter or Other

Title	File
Submission letter from the University of Minnesota Sponsored Projects Administration	e0063d1e-8e5.pdf
Proposal figures	a68e4fc5-c3a.pdf

Administrative Use

Does your project include restoration or acquisition of land rights?

No

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

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?

Yes, Sponsored Projects Administration

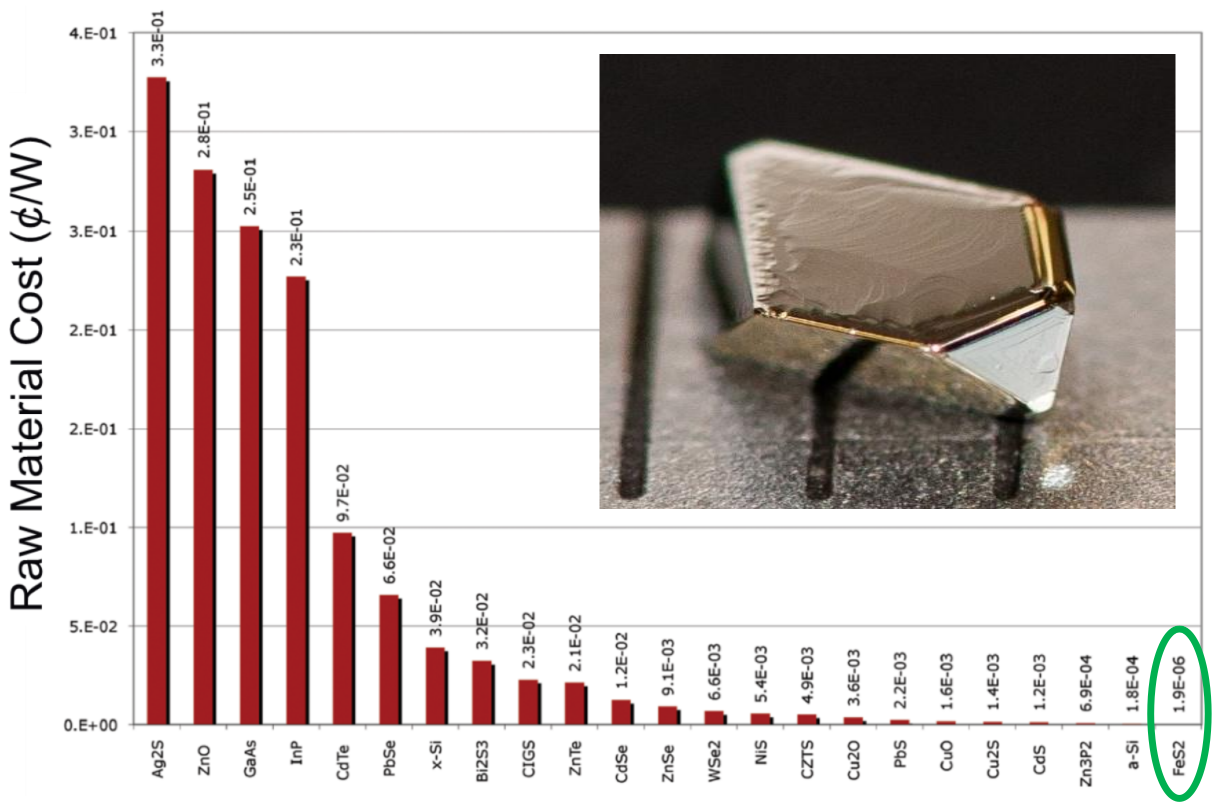

Figure 1: Estimated materials costs (¢ per Watt of power) to produce solar cells at large scale from various photovoltaics. Note iron disulfide (circled green) with 100-times lower cost than its nearest competitor and 10,000-times lower cost than crystalline silicon (from Wadia *et al*., *Environ. Sci. Technol*. **43**, 2072 (2009)). Crystalline Si, the type used in commercial solar cells, is shown here as "x-Si". **Inset:** Synthetic University of Minnesota photovoltaic pyrite crystal.

Figure 2: Left: Sulfur stockpile in Vancouver harbor, Canada. Sulfur is a waste by-product of oil refinement, is thus stockpiled in vast quantities worldwide, and has very low value. **Right:** The MN Mesabi Iron Range. Augmented with capacity from MI, this resource produces approximately 98% of the iron ore used in US steel production.