Rec 10/5/17

3

MTSU Clean Energy Initiative Project Funding Request

There are five (5) sections of the request to complete before submitting. See http://www.mtsu.edu/sga/cleanenergy.shtml for funding guidelines. Save completed form and email to cee@mtsu.edu or mail to MTSU Box 57.

1. General Information	
Name of Person Submitting Request Dr. Keying Ding	
Department/Office Chemistry	Phone # (Office) 615-898-2475
MTSU Box # x68	Phone # (Cell) 615-956-5990
E-mail Keying.Ding@mtsu.edu	Submittal Date 10/02/2017

2. Project Categories (Select One)			
Select the category that best describes the project.			
	Energy Conservation/Efficiency		Sustainable Design
	Alternative Fuels	x	Other research
	Renewable Energy		

3. Project Information
a. Please provide a brief descriptive title for the project. **b.** The project cost estimate is the expected cost of the project to be considered by the committee for approval, which may differ from the total project cost in the case of matching funding opportunities. **Any funding request is a 'not-to-exceed' amount. Any proposed expenditure above the requested amount will require a resubmission.** c. List the source of project cost estimates. d. Provide a brief explanation in response to question regarding previous funding.
3a. Project Title: Bring Green Chemistry on Campus (V)
3b. Project Cost Estimate: $3250 (see attached quote from Aldrich)
3c. Source of Estimate: CHEMICAL VENDERS
3d. If previous funding from this source was awarded, explain how this request differs? This is a new direction of research on alternative and green organic synthesis

by a well-defined molecular catalyst based on an earth-abundant transition metal. Specifically, in this project we will develop an innovative cobalt catalyst system for acceptorless dehydrogenative coupling of primary alcohols to esters.

I am happy to report that an article supported by one previous Clean Energy Fee award has been published in a decent ACS journal. Clean Energy Fee is formally acknowledged in that paper. Follow the link to the article.(**http://pubs.acs.org/doi/abs/10.1021/acs.joc.7b00284**)

4. Project Description

(Completed in as much detail as possible.)

a. The scope of the work to be accomplished is a detailed description of project activities.
b. The benefit statement describes the advantages of the project as relates to the selected project category.
c. The location of the project includes the name of the building, department, and/or specific location of where the project will be conducted on campus.
d. List any departments you anticipate to be involved. Were any departments consulted in preparation of this request? Who? A listing may be attached to this form when submitted.
e. Provide specific information on anticipated student involvement or benefit.
f. Provide information for anticipated future operating and/or maintenance requirements occurring as a result of the proposed project.
g. Provide any additional comments or information that may be pertinent to approval of the project funding request.

4a. Scope: Work to be accomplished

Esters are a family of compounds that are common in organic chemistry and have found ubiquitous applications in chemical, fragrance, and flavor industries. Conventional ester production methods include esterification of carboxylic acids with alcohols, alcoholysis of acyl chlorides and acid anhydrides, carbonylation of alkenes with alcohols, transesterification, etc. Despite these established methods, alternative catalytic acceptorless dehydrogenation of alcohols is an **atom-economical** and **environmentally-friendly** method for synthesis of carbonyl compounds and their derivatives without any oxidants and hydrogen acceptors. This method takes advantage of inexpensive and readily-available alcohols that can be obtained from biomass resources and fermentation. Replacing precious metal catalysts with ones based on first row earth-abundant transition metals is very attractive, which represents one of the most important directions of modern organometallic chemistry in terms of **sustainability**. Our proposed

research just follows the above directions.

In this project, we will develop an innovative non-precious metal cobalt catalyst system for acceptorless dehydrogenative coupling of primary alcohols to afford esters. Our cobalt catalyst is featured with metal-ligand cooperativity (MLC). Normally, ligand does not directly participate in the reactions. In an innovative ligand design with MLC, the ligand is involved in the reaction in a cooperative way with the reactive metal center to facilitate the reaction. Our cobalt catalyst has already shown great activity in dehydrogenation of secondary alcohols and alcohol amine coupling reactions. This project includes three aims: **a**) developing a library of ligands from modular synthesis and their cobalt complexes; **b**) studying their reactivity towards acceptorless dehydrogenative coupling of primary alcohols to esters, including reaction condition optimization and substrate scope exploration; **c**) elucidating the reaction mechanisms via a combined experimental and theoretical approach. Specifically, we will focus on aims **a** and **b** during this funding period. This research will have significant contributions to green chemistry and advanced catalyst design. Student participants will get great hands-on research experience and trainings, which will benefit their future careers in chemistry relevant fields.

The results will serve as important preliminary data for a major grant application to National Science Foundation (NSF) in the near future. A peer-review paper is also expected from this research.

4b. Scope: Benefit Statement

Since joining MTSU in 2013, I have initiated and established a unique "Bring Green Chemistry to MTSU" program aiming to disseminate green and sustainable science and technology and educate the next generation of researchers within the MTSU community, throughout collaborative research, teaching and outreach. Previous and current activities have included: (1) Several ongoing and past research projects in green catalysis supported by MTSU Clean Energy Fee Program, which involve undergraduate and graduate participants; (2) Green chemistry invitational seminars by three well-known US scientists, which are supported by MTSU Distinguished Lecture Fund and Golden Goggle Lectureship. Through these seminars, students have the opportunity to learn what's going on in these cutting-edge research areas and broaden their views; (3) Green chemistry demos and presentations in National ACS meetings, Southeastern ACS regional meetings, Discovery Center at Murfree Spring, and university and local fairs such as Expanding Your Horizons (EYH) supported by WISTEM (participants are K-12 school girls), new Science Building events (participants are from local elementary schools) and Earth Day posters (open to the MTSU community), etc.; (4) Introduction of a "Green Moments" section in General Chemistry courses (I and II). I

incorporate civic engagement in teaching by advocacy of green chemistry concepts and principles. In the General Chemistry classes, I address critical sustainability problems such as global warming and ocean acidification, which are closely related to the topics of the lecture. These "Green Moments" use real-world contexts to teach more complicated concepts in General Chemistry; (5) Advocate to replace common plastic wares and cups with renewable and biodegradable PLA based ones at the MTSU Student Union food court. We drafted a letter to the President of MTSU and hope that the University can pay attention. (6) I integrate concepts of green chemistry into Intermediate Inorganic Chemistry and Foundations of Inorganic Chemistry Aq: Aqueous and Bio-inorganic Chemistry courses. I am also planning to integrate one of my current green chemistry relevant research (supported by NSF) into the General Chemistry (II) course; (7) I serve as the faculty co-advisor to the MTSU Chemistry Society, which is an undergraduate student organization that seeks to increase public interest in chemistry and provide social networking for students with an interest in science. With the great efforts from student members, the MTSU Chemistry Society has won 2015 and 2016 ACS Green Chemistry Student Chapter Award. I believe that with continuous efforts, "Bring Green Chemistry on Campus" program can advance to the next level!

4. Project Description (continued)

4c. Location of Project (Building, etc.)

SCI 3021

4d. Participants and Roles

Keying Ding, PI: supervise the project

Bedraj Pandey, graduate researcher: perform the experiments

David Tyer, undergraduate researcher: perform the experiments

4e. Student participation and/or student benefit

Experiments carried out in this project are advanced synthesis involving air free techniques and product separations and purifications. This project will offer great hands-on research experience and training for students, which will benefit their future careers in chemistry and energy relevant fields.

4f. Future Operating and/or Maintenance Requirements

N/A

4g. Additional Comments or Information Pertinent to the Proposed Project

N/A

5. Project Performance Information

Provide information if applicable.

a. Provide information on estimated annual energy savings stated in units such as kW, kWh, Btu, gallons, etc.
b. Provide information on estimated annual energy cost savings in monetary terms.
c. Provide information on any annual operating or other cost savings in monetary terms. Be specific.
d. Provide information about any matching or supplementary funding opportunities that are available. Identify all sources and explain.

5a. Estimated Annual Energy Savings (Estimated in kW, kWh, Btu, etc.)

N/A

5b. Annual Energy COST Savings ($)

N/A

5c. Annual Operating or Other Cost Savings. Specify. ($)

N/A

5d.Matching or Supplementary Funding (Identify and Explain)

N/A

SIGMA-ALDRICH

Order Preview(This order has not been submitted)

Web Copy

Order Date:2017-10-05 **Purchase Order:** **Payment Term:Prepaid - 1 day net**	**Email order confirmations to:**

Subtotal:3,196.20 USD
Ice/Special Packaging Charges:54.00 USD
Order Total:3,250.20 USD

Line	Product Number	Description	Qty	Your Reference	Your Price	Net Price
000010	337773-25G	CHLORODIISOPROPYLPHOSPHINE, 96%	1		177.00	177.00
		1 In Stock from MILWAUKEE 10/05/17				
000020	481408-5G	CHLORODICYCLOHEXYLPHOSPHINE, 97%	1		249.50	249.50
		1 In Stock from MILWAUKEE 10/05/17				
000030	362891-5G	DIETHYLPHOSPHORAMIDOUS DICHLORIDE, 97%	1		67.90	67.90
		1 In Stock from MILWAUKEE 10/05/17				
000040	39030-100ML	N,N-DIMETHYLETHYLENEDIAMINE, >=98.0% (G&	1		91.60	91.60
		1 In Stock from MILWAUKEE 10/05/17				
000050	D158003-100G	N,N-DIMETHYLETHYLENEDIAMINE, 95%	1		93.60	93.60
		1 In Stock from MILWAUKEE 10/05/17				
000060	127019-25G	N-METHYLETHYLENEDIAMINE, 95%	1		219.00	219.00
		1 : Estimated to ship on 11/30/17				
000070	D39002-100G	1,2-DIBROMOBENZENE, 98%	1		216.00	216.00
		1 In Stock from MILWAUKEE 10/05/17				
000080	186171-4X100ML	N-BUTYLLITHIUM SOLUTION, 1.6 M IN HEXAN&	1		147.00	147.00
		1 In Stock from MILWAUKEE 10/05/17				
000090	215813-75G	POTASSIUM HYDRIDE, 30 WT. % DISPERSION &	1		158.50	158.50
		1 : Estimated to ship on 11/30/17				
000100	184268-25G	4-TERT-BUTYLBENZYL ALCOHOL, 98%	1		133.00	133.00
		1 In Stock from MILWAUKEE 10/05/17				
000110	188212-5G	3-METHYLBENZYL ALCOHOL, 98%	1		29.20	29.20
		1 In Stock from MILWAUKEE 10/05/17				
000120	184268-25G	4-TERT-BUTYLBENZYL ALCOHOL, 98%	1		133.00	133.00
		1 In Stock from Alternate Warehouse 10/06/17				
000130	191639-5G	2,4,6-TRIMETHYLBENZYL ALCOHOL, 99%	1		70.80	70.80
		1 In Stock from MILWAUKEE 10/05/17				
000140	190489-5G	2,4,5-TRIMETHOXYBENZYL ALCOHOL, 97%	1		83.00	83.00
		1 In Stock from MILWAUKEE 10/05/17				
000150	159638-25G	2,4-DIMETHOXYBENZYL ALCOHOL, 99%	1		134.00	134.00
		1 In Stock from MILWAUKEE 10/05/17				
000160	D133000-25G	3,4-DIMETHOXYBENZYL ALCOHOL, 96%	1		44.30	44.30
		1 In Stock from MILWAUKEE 10/05/17				
000170	185701-100G	BENZYLAMINE, REAGENTPLUS, 99%	1		25.80	25.80
		1 In Stock from MILWAUKEE 10/05/17				
000180	M11103-25G	4-METHOXYBENZYLAMINE, 98%	1		55.90	55.90
		1 In Stock from MILWAUKEE 10/05/17				

000190	162493-5G	4-FLUOROBENZYLAMINE, 97%	1		18.70	18.70
		1 In Stock from MILWAUKEE 10/05/17				
000200	263508-1G	4-(TRIFLUOROMETHYL)BENZYLAMINE, 97%	2		25.60	51.20
		2 In Stock from MILWAUKEE 10/05/17				
000210	263494-5G	3-(TRIFLUOROMETHYL)BENZYLAMINE, 98%	1		56.60	56.60
		1 In Stock from MILWAUKEE 10/05/17				
000220	159891-1G	3-METHOXYBENZYLAMINE, 98%	2		42.20	84.40
		2 In Stock from MILWAUKEE 10/05/17				
000230	162485-1G	2-FLUOROBENZYLAMINE, 96%	1		30.10	30.10
		1 In Stock from MILWAUKEE 10/05/17				
000240	127167-5G	3-CHLOROBENZYLAMINE, 98%	1		64.30	64.30
		1 In Stock from MILWAUKEE 10/05/17				
000250	479152-1G	4-BROMOBENZYLAMINE, 96%	1		75.50	75.50
		1 In Stock from MILWAUKEE 10/05/17				
000260	186198-4X100ML	TERT-BUTYLLITHIUM, 1.7M SOLUTION &	1		182.50	182.50
		1 In Stock from MILWAUKEE 10/05/17				
000270	577014-100ML	LITHIUM BIS(TRIMETHYLSILYL)AMIDE 1 M SO&	1		150.50	150.50
		1 In Stock from MILWAUKEE 10/05/17				
000280	442585-100ML-A	PENTAFLUOROPHENYLMAGNESIUM BROMIDE, &	1		166.50	166.50
		1 In Stock from MILWAUKEE 10/05/17				
000290	639052-50ML	3,5-BIS(TRIFLUOROMETHYL)PHENYLMAGNESIUM	2		93.40	186.80
		2 In Stock from MILWAUKEE 10/05/17				