# **List of Suggested Reviewers or Reviewers Not To Include (optional)**

		<b>.</b>	
SUGGESTED REVIEWERS: Not Listed			
REVIEWERS NOT TO INCL Not Listed	UDE:		

The following information regarding collaborators and other affiliations (COA) must be separately provided for each individual identified as senior project personnel. The COA information must be provided through use of this COA template.

Please complete this template (e.g., Excel, Google Sheets, LibreOffice), save as .xlsx or .xls, and upload directly as a Fastlane Collaborators and Other Affiliations single copy doc. Do not upload .pdf.

If there are more than 10 individuals designated as senior project personnel on the proposal, or if there are print preview issues, each completed template must be saved as a .txt file [select the Text (Tab Delimited) option] rather than as an .xlsx or .xls file. This format will still enable preservation of searchable text and avoid delays in processing and review of the proposal.

Please note that some information requested in prior versions of the PAPPG is no longer requested. THIS IS PURPOSEFUL AND WE NO LONGER REQUIRE THIS INFORMATION TO BE REPORTED. Certain relationships will be reported in other sections (i.e., the names of postdoctoral scholar sponsors should not be reported, however if the individual collaborated on research with their postdoctoral scholar sponsor, then they would be reported as a collaborator). The information in the tables is not required to be sorted, alphabetically or otherwise.

There are five separate categories of information which correspond to the five tables in the COA template:

#### **COA template Table 1:**

List the individual's last name, first name, middle initial, and organizational affiliation (including considered affiliation) in the last 12 months.

#### **COA template Table 2:**

List names as last name, first name, middle initial, for whom a personal, family, or business relationship would otherwise preclude their service as a reviewer.

#### COA template Table 3:

List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following:

- The individual's Ph.D. advisors; and
- All of the individual's Ph.D. thesis advisees.

#### **COA template Table 4:**

List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following:

- Co-authors on any book, article, report, abstract or paper with collaboration in the last 48 months (publication date may be later); and
- Collaborators on projects, such as funded grants, graduate research or others in the last 48 months.

#### **COA template Table 5:**

List editorial board, editor-in chief and co-editors with whom the individual interacts. An editor-in-chief must list the entire editorial board.

- Editorial Board: List name(s) of editor-in-chief and journal in the past 24 months; and
- Other co-Editors of journal or collections with whom the individual has directly interacted in the last 24 months.

The template has been developed to be fillable, however, the content and format requirements must not be altered by the user. This template must be saved in .xlsx or .xls format, and directly uploaded into FastLane as a Collaborators and Other Affiliations Single Copy Document. Using the .xlsx or .xls format will enable preservation of searchable text that otherwise would be lost. It is therefore imperative that this document be uploaded in .xlsx or .xls only. Uploading a document in any format other than .xlsx or .xls may delay the timely processing and review of the proposal.

This information is used to manage reviewer selection. See Exhibit II-2 for additional information on potential reviewer conflicts.

- 1 Note that graduate advisors are no longer required to be reported.
- 2 Editorial Board does not include Editorial Advisory Board, International Advisory Board, Scientific Editorial Board, or any other subcategory of Editorial Board. It is limited to those individuals who perform editing duties or manage the editing process (i.e., editor in chief).

List names as Last Name, First Name, Middle Initial. Additionally, provide email, organization, and department (optional) Fixed column widths keep this sheet one page wide; if you cut and paste text, set font size at 10pt or smaller, and To insert *n* blank rows, select *n* row numbers to move down, right click, and choose Insert from the menu.

You may fill-down (crtl-D) to mark a sequence of collaborators, or copy affiliations. Excel has arrows that enable sorting. For "Last Active Date" and "Last Active" columns dates are optional, but will help NSF staff easily determine which information remains relevant for reviewer selection.

"Last Active Date" and "Last Active" columns may be left blank for ongoing or current affiliations.

<u>Table 1:</u> List the individual's last name, first name, middle initial, and organizational affiliation (including considered affiliation) in the last 12 months.

1	Your Name:	Your Organizational Affiliation(s), last 12 r	Last Active Date
	Dera, Przemyslaw K	University of Hawaii	2/6/2018

<u>Table 2:</u> List names as last name, first name, middle initial, for whom a personal, family, or business relationship would otherwise preclude their service as a reviewer.

R: Additional names for whom some relationship would otherwise preclude their service as a reviewer.

to disambiguate common names

2	Name:	Organizational Affiliation	Optional (email, Department)	<b>Last Active</b>

<u>Table 3:</u> List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following.

- G: The individual's Ph.D. advisors; and
- T: All of the individual's Ph.D. thesis advisees.

to disambiguate common names

3	Advisor/Advisee Name:	Organizational Affiliation	Optional (email, Department)		
G:	Katrusiak, Andrzej	Adam Mickiewicz University, Poznan, Poland			

G:	Fingel, Larry W.	Carnegie Institution of Washington	
G:	Prewitt, Charles T.	University of Arisona	
T:	Ehm, Lars	Stony Brook University	
T:	Lavina, Barbara	University of Nevada	

# Table 4: List names as last name, first name, middle initial, and provide organizational affiliations, if known, for the following:

- A: Co-authors on any book, article, report, abstract or paper with collaboration in the last 48 months (publication date may be later); and
- C: Collaborators on projects, such as funded grants, graduate research or others in the last 48 months.

to disambiguate common names

4	Name:	Organizational Affiliation	Optional (email, Department)	Last Active
A:	Achilles, Cherie	University of Indiana Bloomington		2/6/18
A:	Adali, Sibel	Rensselaer Polytechnic Institute		2/6/18
A:	Ahuja, Rajeev	University of Uppsala		2/6/18
A:	Amentrout, Matthew	UCLA		2/6/18
A:	Amulele, George	University of Hawaii		2/6/18
A:	Barkley, Madison	University of Arizona Tucson		2/6/18
A:	Bass, Jay	University of Illinois Urbana Champaign		2/6/18
A:	Beckett, John	Caltech		2/6/18
A:	Bina, Craig	Northwestern University		2/6/18
A:	Bish, David	University of Indiana Bloomington		2/6/18
A:	Blake, David	NASA Ames		2/6/18
A:	Bristow, Thomas	NASA Ames		2/6/18
A:	Broker, Sally	University of Otago		2/6/18
A:	Brown, David	University of Colorado Boulder		2/6/18
A:	Campbell, Andrew	University of Chicago		2/6/18
A:	Caracas, Razvan	University of Lyon		2/6/18
A:	Carbotte, Suzanne	Columbia University		2/6/18
A:	Catalli, Krystle	MIT		2/6/18
A:	Chang, Yin-Yuan	Northwestern University		2/6/18
A:	Chen, Bin	University of Hawaii		2/6/18
A:	Chipera, Steven	LANL		2/6/18
A:	Chow, Paul	Carnegie Institution		2/6/18
A:	Clark, Simon	Macquarie University		2/6/18
A:	Cynn, Honchae	LLNL		2/6/18
A:	DeCarli, Richard	Arizona State University		2/6/18
A:	Depmeier, Wulf	Kiel University		2/6/18
A:	Doak, Jeffrey	Northwestern University		2/6/18
A:	Downs, Robert	University of Arizona Tucson		2/6/18
A:	Dubrovinskaia, Natalia	Bayerisches Geoinstitute		2/6/18
A:	Dubrovinsky, Leonid	Bayerisches Geoinstitute		2/6/18
A:	Duffy, Thomas	Princeton University		2/6/18
A:	Ehm, Lars	Stony Brook University		2/6/18
A:	Evans, William	LLNL		2/6/18
A:	Ferrini, Vicky	Columbia University		2/6/18

A:	Finger Lorm,	Carnagia Institution of Machineton	2/6	6/18
A:	Finger, Larry	Carnegie Institution of Washington		5/18
A:	Finkelstein, Gregory	Caltech		5/18
A:	Fischer, Rebecca	University of Chicago		5/18
A:	Frost, Daniel	Bayerisches Geoinstitute		5/18
_	Gao, Lili	University of Illinois		
A:	Gatta, Diego	University of Milan Carnegie Institution		5/18
A:	Goncharov, Alexander		5/18	
A:	Gong, Jue	Northern Illinois University		5/18
A:	Grubor-Urosevic, Ognje	<u> </u>		5/18
A:	Gupta, Amarnath	San Diego Superercomputing Center		5/18
A:	Gwen, Jacobs	University of Hawaii		5/18
A:	Hauri, Eric	Carnegie Institution		5/18
A:	Heinz, Dion	University of Chicago		5/18
A:	Hellebrand, Eric	University of Hawaii		5/18
A:	Hemley, Russell	Carnegie Institution		5/18
A:	Hilairet, Nadege	University of Lille	2/6	5/18
A:	Holl, Christopher	Princeton University	2/6	5/18
A:	Hope , Ishii	University of Hawaii	2/6	5/18
A:	Hsu, Leslie	Columbia University	2/6	5/18
A:	Hu, Yi	University of Hawaii	2/6	6/18
A:	Hu , Quingyang	HPSTAR	2/6	5/18
A:	Hushur, Anwar	University of Hawaii	2/6	5/18
A:	Irmen, Peyton	University of Chicago	2/6	5/18
A:	Issa, A.	Northwestern University	2/6	5/18
A:	Jackson, Jennifer	Caltech	2/6	5/18
A:	Jacobsen, Steven	Northwestern University	2/6	5/18
A:	Jahn, Sandro	GFZ Potsdam	2/6	5/18
A:	Jameson, Geoffrey	Massey University	2/6	5/18
A:	Joanne, Stubbs	University of Chicago	2/6	6/18
A:	Kantor, Anastasia	ESRF	2/6	5/18
A:	Kantor, Innokenty	ESRF	2/6	5/18
A:	Katrusiak, Andrzej	Adam Mickiewicz University	2/6	5/18
A:	Katsura, Tomo	Bayerisches Geoinstitute	2/6	5/18
A:	Kerstin, Lehnert	Columbia University	2/6	5/18
A:	Kiefer, Boris	New Mexico State University		5/18
A:	Kiefer, Boris	New Mexico State University	2/6	5/18
A:	Kim, Eunja	University of Nevada Las Vegas		5/18
A:	Kirklin, S.J.	Northwestern University		5/18
A:	Knight, Jason	LBNL		5/18
A:	Knorr, Karsten	Bruker AXS		5/18
A:	Kong, Liping	HPSTAR		5/18
A:	Koo, B.	Argonne National Lab		5/18
A:	Krylova, Galina	Argonne National Lab		5/18
A:	Kung, Jennifer	National Cheng Kung Univ.		5/18
A:	Kurnosov, Aleksander	Bayerisches Geoinstitute		5/18
A:	Kwon, G.	Argonne National Lab		5/18
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A:	Lavina, Barbara	University of Nevada Las Vegas	2/6,	/18
A:	Lazarz, John	Northwestern University	2/6,	/18
A:	Lee, B.	Argonne National Lab	2/6,	
A:	Leinenweber, Kurt	Arizona State University	2/6/	
	Li, Jie	University of Michigan Ann Arbor	2/6/	
Λ: Α:	Liermann, Hans-Peter	DESY	2/6,	
Λ: Α:	Lin, Jung-Fu	University of Texas Austin	2/6/	
A:	Liu, Gang	HPSTAR	2/6/	
	Liu, Zenxian	Carnegie Institution of Washington	2/6,	
A:	Liu, Yang	JPL	2/6,	
A:	Lonappan, Dayna	University of Hawaii	2/6,	
A:	Lord, Oliver	Bristol University	2/6,	
A:	Lou, X.	Northwestern University	2/6,	
A:	Ma, Chi	Caltech	2/6,	
Λ: Α:	Manghnani, Murli	University of Hawaii	2/6,	
A:	Mao, Ho-Kwang	Carnegie Institution	2/6,	
A:	Mao, Wendy	Stanford University	2/6,	
	Mao, Zhu	University of Texas Austin	2/6,	
	McCammon, Catherine	Bayerisches Geoinstitutes	2/6,	
A:	McDowell, Alastair	LBNL	2/6,	
	Meng, Yue	Carnegie Institution	2/6,	
A:	Merino, M.	Northwestern University	2/6,	
A:	Miller, N.A.	University of Chicago	2/6,	
A:	Miller, Reece	University of Otago	2/6,	
	Minch, Robert	Kiel University	2/6,	
	Morgenroth, Wolfgang	University of Frankfurt	2/6,	
		Victoria University of Wellington	2/6,	
	Nestola, Fabrizio	University of Padova	2/6,	
	Newville, Matthew	University of Chicago	2/6,	
A:	Nisar, Jawad	University of Uppsala		, 5/18
A:	Oganov, Artem	Stony Brook University	2/6,	
A:	Panero, Wendy	Iowa State University	2/6,	
A:	Parise, John	Stony Brook University	2/6,	
A:	Peters, Lars	Kiel University	2/6,	
A:	Petitgirard, S.	DESY	2/6,	
A:	Plonka, Anna	Stony Brook University	2/6,	
A:	Podsiadlo, Paul	Argonne National Lab	2/6,	
A:	Posner, Esther	Bayerisches Geointitute	2/6,	
A:	Prakapenka, Vitali	University of Chicago	2/6,	
A:	Prewitt, Charles	University of Arizona	2/6,	
	Rainey, Emma	UCLA	2/6,	
A:	Reaman, Daniel	University of Chicago	2/6,	
	Rivers, Mark	University of Chicago	2/6,	
A:	Rossman, George	Caltech	2/6,	
A:	Sarrazin, Philipe	InXitu, Inc.	2/6,	
A:	Schaller, Richard	Argonne National Lab		/18
A:	Schaller, Richard	Argonne National Lab	2/6	,

A:	Cabiford David	LANII	2/6/18
	Schiferl, David	LANL	2/6/18
A:	Sekar, M.	University of Hawaii	2/6/18
A:	Sharp, Thomas	Arizona State University	2/6/18
A:	Shebanova, Olga	Carnegie Institution	2/6/18
_	Shelton, Hannah	University of Hawaii	
_	Shen, Guoyin	Carnegie Institution	2/6/18
	Shevchenko, Elena	Argonne National Lab	2/6/18
A:	Shieh, Sean	Western Ontario University	2/6/18
_	Shim, Sang-Heon	University of Arizona	2/6/18
A:	Shofner, G.A.	Bristol University	2/6/18
A:	Siidra, O.I.	Kiel University	2/6/18
A:	Sinogeikin, Stanislav	Carnegie Institution	2/6/18
A:	Smith, Jesse	Carnegie Institution	2/6/18
_	Somayazulu, Maddury	Carnegie Institution	2/6/18
A:	Soule, Samuel	Woods Hole Oceanogr. Inst.	2/6/18
A:	Spear, Frank	Rensselaer Polytechnic Institute	2/6/18
A:	Speziale, Sergio	GFZ Potsdam	2/6/18
A:	Sturhahn, Wolfgang	Caltech	2/6/18
A:	Sutton, Steven	University of Chicago	2/6/18
A:	Tait, Kimberly	Royal Ontario Museum	2/6/18
A:	Tallon, Feffrey	Victoria University of Wellington	2/6/18
A:	Tang, Yuzhao	Inst. Of Biochemistry, Shanghai	2/6/18
A:	Taylor, Lawrence	Univ. of Tennessee	2/6/18
A:	Thomas, Sylvia-Monique	University of Nevada Las Vegas	2/6/18
A:	Thompson, Richard	University of Arizona Tucson	2/6/18
A:	Timothy, Strobel	Carnegie Institution	2/6/18
A:	Tkachev, Sergey	University of Chicago	2/6/18
A:	Townsend, Joshua	Northwestern University	2/6/18
A:	Tschauner, Oliver	University of Nevada Las Vegas	2/6/18
A:	Vaniman, David	Planetary Science Institute	2/6/18
A:	Wang, Chuanyi	Xinjiang Tech. Inst. of Phys. and Chem.	2/6/18
A:	Weck, Philippe	University of Nevada Las Vegas	2/6/18
A:	Wei, Su-huai	Beijing Comp. Sci. Res. Center	2/6/18
A:	Weidner, Donald	Stony Brook University	2/6/18
A:	Werheit, Helmut	University of Duisburg-Essen	2/6/18
A:	Williams, Quentin	UC Santa Cruz	2/6/18
A:	Wolf, Aaron	University of Michigan	2/6/18
A:	Wolverton, Christopher	Northwestern University	2/6/18
A:	Wu, Zhongqing	Univ. of Sci. and Technology of China	2/6/18
A:	Xiao, Yuming	Carnegie Institution of Washington	2/6/18
	Xie, Z.	Arizona State University	2/6/18
A:	Xu, Tao	Northern Illinois University	2/6/18
A:	Yang, Wenge	Carnegie Institution	2/6/18
A:	Yang, Wenge	HPSTAR	2/6/18
A:	Ye, Yu	University of Colorado Booulder	2/6/18
A:	Zaslavsky, Illia	San Diego Superercomputing Center	2/6/18
	zasiavsky, iiila	Jan Diego Japerer computing Center	2,0,10

A:	Zerr, Andreas	University of Paris Nord	2/6/18
A:	Zhang, Dongzhou	University of Hawaii	2/6/18
A:	Zhang, Jin	University of Hawaii	2/6/18
A:	Zhang, Li	Carnegie Institution	2/6/18
A:	Zhao, J.	Argonne National Lab	2/6/18
A:	Zhao, Yusheng	University of Nevada	2/6/18
A:	Zhu, Kai	Nat. Renew. Energy Lab., Golden	2/6/18
A:	Zhuravlev, Kirill	University of Chicago	2/6/18

Table 5: List editorial board, editor-in chief and co-editors with whom the individual interacts. An editor-in-chief

- B: Editorial Board: List name(s) of editor-in-chief and journal in the past 24 months; and
- E: Other co-Editors of journal or collections with whom the individual has directly interacted in the last 24 months.

to disambiguate common names

5	Name:	Organizational Affiliation	Journal/Collection	<b>Last Active</b>
B:	Weidner, Donald	Stony Brook University	COMPRES Long Range Report	1/1/17
E:				

## COVER SHEET FOR PROPOSAL TO THE NATIONAL SCIENCE FOUNDATION

PROGRAM ANNOUNCEMENT/SOLICITATION NO./DUE DATE			☐ Special Exc	ception to Deadline Date Policy FOR NSF USE ONLY		R NSF USE ONLY			
NSF 17-554					NSF PI	NSF PROPOSAL NUMBER			
FOR CONSIDERATION	BY NSF ORGANIZATION	ON UNIT(	S) (Indicate the	most specific unit know	wn, i.e. program, division, et	c.)			
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\$ 10,000		6	months	`	07/0	1/18	8 IF APPLICABLE		
THIS PROPOSAL INCLU		MS LISTE	ED BELOW			☐ HUMAN SUBJECTS Human Subjects Assurance Number			
☐ DISCLOSURE OF LO					Exemption Subsection or IRB App. Date				
☐ PROPRIETARY & PR	RIVILEGED INFORMAT	ION				L ACTIVITIES: COUN	TRY/COUNTRIES IN	VOLVED	
☐ HISTORIC PLACES ☐ VERTEBRATE ANIM	ALSIACIIC Ann Data								
PHS Animal Welfare	Assurance Number				⊠ COLLABORATI\				
☐ TYPE OF PROPOSA	L Conference				Not a collabo	rative proposal			
PI/PD DEPARTMENT <b>Hawaii Institute</b>	e of Geophys. & l	Planeto		STAL ADDRESS C <b>ampus Roa</b>	d, Box 368				
PI/PD FAX NUMBER			HONG	OLULU, HI	06822224				
808-956-3188				l States	900222234				
NAMES (TYPED)		High D		Yr of Degree	Telephone Numb	er	Email Address	3	
PI/PD NAME			_			_			
Przemyslaw Der	a	DPhi	1	2000	808-956-634	7 pdera@h	awaii.edu		
CO-PI/PD  Dongzhou Zhan	σ	DPhi	1	2015	808-956-780	0 dzhona@	hawaii.edu		
CO-PI/PD	<u> </u>	DI III	1	2013	000-930-760	Uznang@	nawan.cuu		
CO-PI/PD		<u> </u>							
CO-PI/PD									

#### **CERTIFICATION PAGE**

## Certification for Authorized Organizational Representative (or Equivalent) or Individual Applicant

By electronically signing and submitting this proposal, the Authorized Organizational Representative (AOR) or Individual Applicant is: (1) certifying that statements made herein are true and complete to the best of his/her knowledge; and (2) agreeing to accept the obligation to comply with NSF award terms and conditions if an award is made as a result of this application. Further, the applicant is hereby providing certifications regarding conflict of interest (when applicable), drug-free workplace, debarment and suspension, lobbying activities (see below), nondiscrimination, flood hazard insurance (when applicable), responsible conduct of research, organizational support, Federal tax obligations, unpaid Federal tax liability, and criminal convictions as set forth in the NSF Proposal & Award Policies & Procedures Guide (PAPPG). Willful provision of false information in this application and its supporting documents or in reports required under an ensuing award is a criminal offense (U.S. Code, Title 18, Section 1001).

#### **Certification Regarding Conflict of Interest**

The AOR is required to complete certifications stating that the organization has implemented and is enforcing a written policy on conflicts of interest (COI), consistent with the provisions of PAPPG Chapter IX.A.; that, to the best of his/her knowledge, all financial disclosures required by the conflict of interest policy were made; and that conflicts of interest, if any, were, or prior to the organization's expenditure of any funds under the award, will be, satisfactorily managed, reduced or eliminated in accordance with the organization's conflict of interest policy. Conflicts that cannot be satisfactorily managed, reduced or eliminated and research that proceeds without the imposition of conditions or restrictions when a conflict of interest exists, must be disclosed to NSF via use of the Notifications and Requests Module in FastLane.

#### **Drug Free Work Place Certification**

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent), is providing the Drug Free Work Place Certification contained in Exhibit II-3 of the Proposal & Award Policies & Procedures Guide.

#### **Debarment and Suspension Certification**

(If answer "yes", please provide explanation.)

Is the organization or its principals presently debarred, suspended, proposed for debarment, declared ineligible, or voluntarily excluded from covered transactions by any Federal department or agency?

Yes ☐ No 🛛

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) or Individual Applicant is providing the Debarment and Suspension Certification contained in Exhibit II-4 of the Proposal & Award Policies & Procedures Guide.

#### Certification Regarding Lobbying

This certification is required for an award of a Federal contract, grant, or cooperative agreement exceeding \$100,000 and for an award of a Federal loan or a commitment providing for the United States to insure or guarantee a loan exceeding \$150,000.

#### Certification for Contracts, Grants, Loans and Cooperative Agreements

The undersigned certifies, to the best of his or her knowledge and belief, that:

- (1) No Federal appropriated funds have been paid or will be paid, by or on behalf of the undersigned, to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with the awarding of any Federal contract, the making of any Federal loan, the entering into of any cooperative agreement, and the extension, continuation, renewal, amendment, or modification of any Federal contract, grant, loan, or cooperative agreement.
- (2) If any funds other than Federal appropriated funds have been paid or will be paid to any person for influencing or attempting to influence an officer or employee of any agency, a Member of Congress, an officer or employee of Congress, or an employee of a Member of Congress in connection with this Federal contract, grant, loan, or cooperative agreement, the undersigned shall complete and submit Standard Form-LLL, "Disclosure of Lobbying Activities," in accordance with its instructions.
- (3) The undersigned shall require that the language of this certification be included in the award documents for all subawards at all tiers including subcontracts, subgrants, and contracts under grants, loans, and cooperative agreements and that all subrecipients shall certify and disclose accordingly.

This certification is a material representation of fact upon which reliance was placed when this transaction was made or entered into. Submission of this certification is a prerequisite for making or entering into this transaction imposed by section 1352, Title 31, U.S. Code. Any person who fails to file the required certification shall be subject to a civil penalty of not less than \$10,000 and not more than \$100,000 for each such failure.

#### **Certification Regarding Nondiscrimination**

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is providing the Certification Regarding Nondiscrimination contained in Exhibit II-6 of the Proposal & Award Policies & Procedures Guide.

#### **Certification Regarding Flood Hazard Insurance**

Two sections of the National Flood Insurance Act of 1968 (42 USC §4012a and §4106) bar Federal agencies from giving financial assistance for acquisition or construction purposes in any area identified by the Federal Emergency Management Agency (FEMA) as having special flood hazards unless the:

- (1) community in which that area is located participates in the national flood insurance program; and
- (2) building (and any related equipment) is covered by adequate flood insurance.

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) or Individual Applicant located in FEMA-designated special flood hazard areas is certifying that adequate flood insurance has been or will be obtained in the following situations:

- (1) for NSF grants for the construction of a building or facility, regardless of the dollar amount of the grant; and
- 2) for other NSF grants when more than \$25,000 has been budgeted in the proposal for repair, alteration or improvement (construction) of a building or facility.

# Certification Regarding Responsible Conduct of Research (RCR) (This certification is not applicable to proposals for conferences, symposia, and workshops.)

By electronically signing the Certification Pages, the Authorized Organizational Representative is certifying that, in accordance with the NSF Proposal & Award Policies & Procedures Guide, Chapter IX.B., the institution has a plan in place to provide appropriate training and oversight in the responsible and ethical conduct of research to undergraduates, graduate students and postdoctoral researchers who will be supported by NSF to conduct research. The AOR shall require that the language of this certification be included in any award documents for all subawards at all tiers.

## **CERTIFICATION PAGE - CONTINUED**

#### **Certification Regarding Organizational Support**

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is certifying that there is organizational support for the proposal as required by Section 526 of the America COMPETES Reauthorization Act of 2010. This support extends to the portion of the proposal developed to satisfy the Broader Impacts Review Criterion as well as the Intellectual Merit Review Criterion, and any additional review criteria specified in the solicitation. Organizational support will be made available, as described in the proposal, in order to address the broader impacts and intellectual merit activities to be undertaken.

#### **Certification Regarding Federal Tax Obligations**

When the proposal exceeds \$5,000,000, the Authorized Organizational Representative (or equivalent) is required to complete the following certification regarding Federal tax obligations. By electronically signing the Certification pages, the Authorized Organizational Representative is certifying that, to the best of their knowledge and belief, the proposing organization:

- (1) has filed all Federal tax returns required during the three years preceding this certification;
- (2) has not been convicted of a criminal offense under the Internal Revenue Code of 1986; and
  (3) has not, more than 90 days prior to this certification, been notified of any unpaid Federal tax assessment for which the liability remains unsatisfied, unless the assessment is the subject of an installment agreement or offer in compromise that has been approved by the Internal Revenue Service and is not in default, or the assessment is the subject of a non-frivolous administrative or judicial proceeding.

#### **Certification Regarding Unpaid Federal Tax Liability**

When the proposing organization is a corporation, the Authorized Organizational Representative (or equivalent) is required to complete the following certification regarding Federal Tax Liability:

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is certifying that the corporation has no unpaid Federal tax liability that has been assessed, for which all judicial and administrative remedies have been exhausted or lapsed, and that is not being paid in a timely manner pursuant to an agreement with the authority responsible for collecting the tax liability.

#### **Certification Regarding Criminal Convictions**

When the proposing organization is a corporation, the Authorized Organizational Representative (or equivalent) is required to complete the following certification regarding Criminal Convictions:

By electronically signing the Certification Pages, the Authorized Organizational Representative (or equivalent) is certifying that the corporation has not been convicted of a felony criminal violation under any Federal law within the 24 months preceding the date on which the certification is signed.

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Certification Dual Use Research of Concern					
By electronically signing the certification pages, the Authorized Organizational Representative is certifying that the organization will be or is in compliance with all aspects of the United States Government Policy for Institutional Oversight of Life Sciences Dual Use Research of Concern.					
	3				
AUTHORIZED ORGANIZATIONAL REPRESENTATIVE SIGNATUR		SIGNATURE	DATE		
NAME					
TELEPHONE NUMBER	EMAIL ADDRESS		FAX NUMBER		
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## **Project Summary**

#### **Overview:**

This proposal request financial support for participation of 10 early career (graduate student, postdoc or tenure-track faculty) in the 2018 Workshop of the International Union of Crystallography (IUCr) Commission on High Pressure, which will be held in Honolulu Hawaii, from July 29, until August 2, 2018 at the Ala Moana Hotel. 3.5 days of regular conference program will be preceded with a one full day student/postdoc training event on analysis of single crystal X-ray diffraction data at high pressure.

#### **Intellectual Merits:**

Extreme-conditions science is a vibrant, multidisciplinary field that characterizes unique states of matter, simulates processes that take place in inaccessible environments such as planetary interiors, and synthesizes new materials with properties that have compelling technological applications. Understanding of the effect of pressure on minerals and earth forming materials is central to geophysics, mineral physics and planetary science. The interiors of all planetary bodies are built of minerals that exist under high pressure and temperature conditions. Meteorite ejection and impact phenomena involve generation of dynamic shock pressure. Understanding how pressure affects the structure, properties and behavior of minerals enables understanding of global phenomena such as earthquakes, volcanism, plate tectonics, etc. Proper education of the new generation of earth scientists who will study and model properties and processes of planetary interiors is an issue of great importance for the future of geosciences, and represents a significant challenge.

We hope the 2018 Honolulu event and the NSF funding requested here to help advertise the NSF-funded COMPRES (Consortium for Materials Properties Research in Earth Science) synchrotron user facilities, PX^2 at APS and beamline 12.2.2 at ALS to the international high pressure community and new COMPRES users and to inspire new crystallography related research collaborations. The event will emphasize training of young scientists in basic principles of single crystal sample preparation, data collecting and analysis.

#### **Broader Impacts:**

The IUCr Commission on High Pressure over the last decade has been spearheading discussions and efforts aimed at defining experimental data quality standards and best data deposition formats for high pressure crystallography. The 2018 Honolulu Workshop will provide opportunity to familiarize and engage the Mineral Physics community in the United States with these activities.

A number of previous IUCr HP workshops produced published peer-reviewed proceedings. These include the 2009 Workshop in Harbin, China, where the PI served as the IPC chair and coeditor of the special volume of High Pressure Research Journal, where the conference papers were published. We are tentatively planning to use the same journal for publication of the 2018 proceedings.

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Appendix (List below.) (Include only if allowed by a specific program announcement/solicitation or if approved in advance by the appropriate NSF Assistant Director or designee)		
Appendix Items:		

<sup>\*</sup>Proposers may select any numbering mechanism for the proposal. The entire proposal however, must be paginated. Complete both columns only if the proposal is numbered consecutively.

# E<sup>3</sup>: Extreme materials, extreme phenomena, extreme environments

2018 Workshop of the IUCr Commission on High Pressure Honolulu, HI, July 29 – August 2, 2018

#### Introduction

This proposal request financial support for participation of 10 early career (graduate student, postdoc or tenure-track faculty) in the 2018 Workshop of the International Union of Crystallography (IUCr) Commission on High Pressure, which will be held in Honolulu Hawaii, from July 29, until August 2, 2018 at the Ala Moana Hotel. 3.5 days of regular conference program will be preceded with a one full day student/postdoc training event on analysis of single crystal X-ray diffraction data at high pressure.

Extreme-conditions science is a vibrant, multidisciplinary field that characterizes unique states of matter, simulates processes that take place in inaccessible environments such as planetary interiors, and synthesizes new materials with properties that have compelling technological applications. The last decade has seen milestones reached in crystallographic instrumentation for high-pressure studies and improvements in the robustness of experimental methodology and software, as well as ab-initio techniques. Crystallographic structure determination at pressures up to a megabar has become routine, and several recent reports have even far exceeded that pressure. X-ray diffraction is the most direct method to determine sample's crystal structure at high pressures. There are two approaches to carry out diffraction experiment at high pressures, the conventional powder diffraction, and the emerging single crystal diffraction. Similar to the routine powder diffraction technique, single crystal diffraction can provide structural related information of the sample, including lattice parameters, density and equation of states. On the other hand, more knowledge beyond crystal structure can be extracted from single crystal diffraction, such as chemical bonding, anisotropy and lattice dynamics. Single crystal diffraction requires careful sample preparation, sophisticated instrumentation and advanced data analysis software, which increases its entrance barrier in comparison with the straightforward powder diffraction. Though most Earth related materials have been thoroughly studied with powder diffraction, many major components in the mantle and core haven't been systematically measured by single crystal diffraction yet.

Understanding of the effect of pressure on minerals and earth forming materials is central to geophysics, mineral physics and planetary science. The interiors of all planetary bodies are built of minerals that exist under high pressure and temperature conditions. Meteorite ejection and impact phenomena involve generation of dynamic shock pressure. Understanding how pressure affects the structure, properties and behavior of minerals enables understanding of global phenomena such as earthquakes, volcanism, plate tectonics, etc. Proper education of the new generation of earth scientists who will study and model properties and processes of planetary interiors is an issue of great importance for the future of geosciences, and represents a significant challenge. Novel experimental and theoretical methods used in high-pressure research are sophisticated and rarely covered to a satisfactory extent in university curricula. Knowledge and experience is usually acquired by young scientists the hard way – through trial and error. Standard format scientific conferences, while good for the purpose of becoming aware of the latest trends and new results in the discipline, are not best suited to emphasize education and training in efficient and optimized ways. Very few opportunities in geophysics and mineral physics exist for organized training outside of universities that would allow young scientists to efficiently learn from the international experts and establish scientific collaborations. We hope the 2018 event to close this gap.

#### Statement of the necessity

Extreme crystallography is a fast-developing research field. For example, the NSF has been supporting (through COMPRES Cooperative agreement) the scientific program of Partnership for eXtreme Xtallography (PX^2) since 2015. PX^2 is providing new capabilities for high-pressure diamond anvil cell research at the GeoSoilEnviroCARS beamline of the Advanced Photon Source (APS), Argonne National Laboratory. By February 2018, the PX^2 program has hosted more than 150 groups of users, and 21 peer-reviewed papers from PX^2 users have been published or accepted, about ¼ of which were in high profile journals (1 Nature, 1 Science, 2 PNAS and 1 Nature Communications).

# Number of PX^2 general users

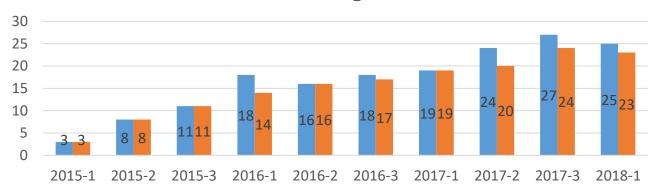


Fig. 1: Statistics of PX^2 general user operation for each APS operational run. Blue bars show the total number of general users who applied for beamtime and wanted to carry out high pressure crystallography experiments, and red bars show the number of general users who were granted beamtime and could carry out their high pressure crystallography experiments.

Similarly successful program offering single-crystal high pressure experimental capabilities, also sponsored by COMPRES, has recently been implemented at beamline 12.2.2 of the Advanced Light Source, at Lawrence Berkeley National Laboratory.

On the other hand, though the demand for high pressure crystallography is increasing, a significant amount of high pressure researchers still have quite limited access to this powerful technique. Those researchers either haven't heard about high pressure single crystal diffraction before, or lack knowledge in preparing the optimal samples for crystallographic experiments, or have insufficient training in the data analysis. We have been providing high pressure crystallography training to all of the PX^2 users, who represent a significant portion of current high-pressure crystallography researchers in the US. However, our training can only be provided when the users are on-site, performing the experiment, which is quite inefficient. Considering the fact that the most recent high pressure crystallography workshop in the US was held in 2010, the need to attract and cultivate next generation of high pressure crystallography researchers in the US is urgent. Therefore, we believe that it is necessary to hold this workshop.

The IUCr Commission on High Pressure over the last decade has been spearheading discussions and efforts aimed at defining experimental data quality standards and best data deposition formats for high pressure crystallography. The 2018 Honolulu Workshop will provide opportunity to familiarize and engage the Mineral Physics community in the United States with these activities.

## **History of IUCr High Pressure Workshops**

The IUCr is an International Scientific Union. Its objectives are to promote international cooperation in crystallography and to contribute to all aspects of crystallography, to promote international publication of crystallographic research, to facilitate standardization of methods, units, nomenclatures and symbols, and to form a focus for the relations of crystallography to other sciences.

At the 14th Congress of IUCr in Perth, Australia in 1987, a High-Pressure Group was established within the Commission on Crystallographic Apparatus, to represent and support high-pressure crystallography. The subsequent decade saw an extraordinary growth in the range and quality of high-pressure diffraction studies – particularly using powder methods – on both synchrotron and neutron sources. This was stimulated by the power of present-day sources, and by major developments in detectors and high-pressure technology. The High-Pressure Group maintained a high level of activity from its inception, with a series of international workshops, starting in Munich in 1989. This lead to establishment of the current Commission on High Pressure at the XVII IUCr Congress in Seattle, USA. The PI, Dera served as chair of the IUCr HP Commission from 2008 until 2014, and chaired the International Program Committees of 4 previous IUCr HP workshops.

The IUCr HP Commission has been organizing regular annual workshops each year since 1997, except for the years of IUCr Congresses. The 2018 Honolulu workshop will be the 15th event in this series. A list of the previous workshops is included below:

1997 HP Workshop, ESRF Grenoble, France

1998 HP Workshop, APS Chicago, USA

1999 XVIII IUCr Congress in Glasgow, UK

2000 HP Workshop, SPring-8 Japan

2001 HP Workshop, LURE Orsay, France

2002 XIX IUCr Congress, Geneva, Switzerland

2003 HP Workshop, ALS Berkeley, USA

2004 HP Workshop, CLS Saskatoon, Canada

2005 XX IUCr Congress, Florence, Italy

2006 HP Workshop, DELSY Dubna, Russia

2007 HP Workshop, Oxford, UK

2008 XXI IUCr Congress, Osaka, Japan

2009 HP Workshop, Harbin, China

2010 HP Workshop, Gatlinburg, USA

2011 XXII IUCr Congress, Madrid, Spain

2012 HP Workshop, Mito, Japan

2013 HP Workshop, DESY Hamburg, Germany

2014 XXIII IUCr Congress, Montreal, Canada

2015 HP Workshop, LNLS Campinas, Brasil

2016 HP Workshop, PAL Pohang, Korea

2017 XXIV IUCr Congress, Hyderabad, India

2018 HP Workshop, Honolulu, USA

## **Organizing Committees**

The local organization of the 2018 IUCr HP Workshop in Honolulu is lead by a five-person committee, chaired by the PI, Dera. List of Local Organizing Committee members is included below:

Przemyslaw Dera, University of Hawaii at Manoa, Chair Vitali Prakapenka, University of Chicago Bin Chen, University of Hawaii at Manoa Dongzhou Zhang, University of Hawaii at Manoa Gregory Finkelstein, University of Hawaii at Manoa

### **International Program Committee (IPC)**

The programmatic leadership over the scope and content of the 2018 Workshop is overseen by a 16 person committee, representing 11 countries:

H. Liu (Chair, People's Republic of China)

N.M. Souza-Neto (Brazil)

B. Zakharov (Russia)

N. Dubrovinskaia (Germany)

N. Garg (India)

K.F. Dziubek (Italy)

S. Moggach (UK)

Y. Ohishi (Japan)

J.-P. Itié (France)

G. Shen (USA)

R. Angel (Italy)

S. Klotz (France)

A. Lazicki (USA)

M. McMahon (UK)

J. Parise (USA)

A. Katrusiak (Poland)

#### Dissemination

The 2009 Erice ISC has a working website located at:

https://hp2018honolulu.github.io/organizers.html

The website provides basic information about the venue, lecturers, day-by-day schedule, etc. The meeting registration and abstract submission opened on March 15, 2018.

Meeting announcements were distributed using the mailing lists of COMPRES, Mineralogical Society of America, and AIRAPT (International Association for the Advancement of High Pressure Science and Technology).

A number of previous IUCr HP workshops produced published peer-reviewed proceedings. These include the 2009 Workshop in Harbin, China, where the PI served as the IPC chair and co-editor of the special volume of High Pressure Research Journal, where the conference papers were published. We are tentatively planning to use the same journal for publication of the 2018 proceedings.

## Total meeting budget and other than NSF sources of funding

The meeting cost calculation is based on the assumption of 100 registered participants, with 50:50 distribution of regular and student attendees, which is consistent with historical trends at earlier events of the same series. The total cost of the meeting is estimated at about \$70,000. This cost includes all expenses related to the one day pre-conference training event, meeting room and audiovisual equipment fees, meals (breakfast and lunch) and coffee breaks for all participants, Welcome Reception, Conference Dinner, and Poster Session. The attendees will have to cover the cost of hotel accommodations by themselves. In addition to the accommodations at the main Workshop venue, the Ala Moana Hotel, we also arranged a set of affordable rooms to be reserved at the University of Hawaii East-West Center, to provide housing options for attendees on more constrained budget.

The financing for the workshop relies at about 70% on registration fees (\$600 regular participant, \$400 student). University of Hawaii allocated a budget of \$8,000 to help offset the meeting costs. We were also able to secure \$5,000 from commercial sponsors and \$5,000 from HPCAT and GSECARS, two national user facilities serving mineral physics community. A request for workshop support at \$22,775 was also submitted to COMPRES, but the Consortium has not been able to reach a funding decision at the time of the submission of this proposal.

The IUCr HP workshops typically offer young participant travel awards, which are meant to offset the participation cost for students, postdocs and young, untenured faculty. In 2018 we are planning to follow this tradition. A call for applications for such support has been posted on the Workshop website, with a deadline of April 15. The submitted applications will be evaluated by a 6-person Committee consisting of the local organizers and the chair of the IPC. We are planning to offer \$1,000 travel awards which will cover the registration fee and portion of the travel expenses. The funds requested within this proposal will also be distributed as young participant travel awards (10 awards at \$1,000 each), but will be restricted to applicants affiliated with academic or research institutions in the United States.

### Preliminary program

The main part of the IUCr workshop will be 3.5 days long, and will feature 11 scientific sessions, covering a multidisciplinary range of topics within high pressure science. List of session titles and session chair is included below. Each session is expected to be 2-2.5h long and consist of 4-6 talks.

- Session 1: Molecules under pressure (Chair: Christos Lampropoulos)
- Session 2: Advanced synchrotron and optical characterization of materials at extreme conditions (Chairs: Vitali Prakapenka and Dongzhou Zhang)
- Session 3: New frontiers in extreme conditions crystallography (Chairs: Amy Lazicki and David McGonegle)
- Session 4: High pressure chemistry and synthesis (Chair: Kamil Dziubek)
- Session 5: Materials science (Chair: Haozhe Liu and Nenad Velisavljevic)
- Session 6: Materials metastability under pressure (Chair: Guoyin Shen and Peter Lazor)
- Session 7: High-pressure crystallography in earth and planetary science (Chair: Jiuhua Chen and Bin Chen)
- Session 8: Electronic and magnetic materials at extreme conditions (Chairs: Narcizo Souza-Neto and Yang Ding)
- Session 9: Coordination chemistry and porous materials (Chair: Andrzej Katrusiak) and John Parise
- Session 10: Computational approaches in extreme conditions science (Chairs: Zhongquing Wu and John Tse)
- Session 11: Emerging experimental techniques (Chair: Nandini Garg)

## **Keynote speakers**

The workshop will include 3 keynote talks, by Dr. Jon Eggert (LANL, USA), Dr. Yongjae Lee (Yonsei University, Korea), and Dr. Shanti Demmya hort biographical notes of the keynote speakers are included below.

Jon Eggert received his B.S. degree in Physics in 1985 from Montana State University, and his Ph.D. in Physics in 1991 from Harvard University. His thesis research focused on pressure-induced insulator-metal transitions in xenon and hydrogen. In 1991 he worked as a postdoctoral fellow at the Institute of Physics, Chinese Academy of Sciences, Beijing, implementing an optical laboratory for diamond-anvil cell (DAC) studies. In 1992 he began a postdoctoral fellowship at the Carnegie Institution of Washington, Geophysical Laboratory in Washington, DC, concentrating primarily on studies of the solid hydrogens at very high pressure. Dr. Eggert was an assistant professor at Pomona College in Claremont, CA for two years beginning in 1994. He moved to the Colorado School of Mines (CSM), Golden CO in 1996. As a professor, Dr. Eggert continued to work on high pressure physics as well as broadening into the study of granular materials. In 1999, he took a two-year leave of absence to work at the Commissariat a l'Energie Atomique (CEA) near Paris France. At the CEA, Dr. Eggert developed a highly-accurate method for measuring x-ray diffraction of liquids in the DAC. In 2001 Dr. Eggert joined the Laser Shock Equation of State (EOS) group at Lawrence Livermore National Laboratory (LLNL) in Livermore, CA. At LLNL, he has worked on: coupling laser-generated shock waves into DACs to study He, H2 and D2 along alternate Hugoniots; analysis of isentropic compression experiment (ICE) EOS; phase transitions in shocks and ramp drives; melting of diamond; and anisotropic shock propagation in single crystals.

Yongjae Lee is a professor at the Department of Earth System Sciences, Yonsei University in Korea and an adjunct staff scientist at HPSTAR in China. With Ph.D. in crystallography from Stony Brook University in 2001, he discovered a "super-hydrated zeolite" under pressure while working as a postdoctoral fellow at Brookhaven National Laboratory. Through joining Yonsei University in 2006, he has continued to understand high-pressure behaviors of porous materials and to design novel chemistry and possible usages. Recently, he extended his research interests into global problems and reported "super-hydrated clay" forming under moderate pressure and temperature conditions, which bears strong implications in water transport into the mantle and seismicity and volcanism along the subduction zones. He has been actively engaged in developing specialized high-pressure programs at Stanford Synchrotron Radiation Lightsource and Pohang Accelerator Laboratory including dynamic compression using short pulse laser at PAL-XFEL. Yongjae Lee is the recipient of Alvin Van Valkenburg award from Gordon Conference and Sidhu award from Pittsburgh Diffraction Conference in 2002 and the author of more than 150 research papers.

Shanti Deemyad, an Associate Professor of Physics and Astronomy at the University of Utah, recently helped solve a long-standing mystery about lithium, the first element in the periodic table that is metallic at ambient conditions. Lithium, which is a key element in electronics and battery technology, has played an important role in the development of modern condensed matter theories. The crystal structure of materials at zero pressure and temperature is one of their most basic properties. Until now, it was thought that a complex arrangement of lithium atoms, observed during cooling in the laboratory, was its lowest energy state. But the idea baffled theoretical physicists since lithium has only three electrons and therefore should have a simple atomic structure. Deemyad's new study combined theory and experimentation to discover the true structure of lithium in its lowest energy state at cold temperatures. Deemyad joined the faculty as an assistant professor of physics and astronomy in 2010. Her lab is divided in two major areas: quantum solids and highly correlated electron systems with an emphasis on studying the nature of electronic interactions; and high pressure guided synthesis of materials with new or enhanced properties for energy storage and transport.

## One day High Pressure Single Crystal Data Analysis Training Event on July 29, 2018

The purpose of this training event will be to introduce single crystal diffraction capabilities and methodology currently available at the Partnership for eXtreme Xtallography (PX^2), a dedicated high pressure crystallography user program hosted by GSECARS at Argonne National Lab, and funded by COMPRES and well as COMPRES beamline 12.2.2 at the Advanced Light Source in Berkeley, and educate students and early-career scientists about single crystal diffraction with extensive hands-on training.

Workshop motivation: Single crystal diffraction is one of the most direct methods to determine sample's crystal structure at high pressures. Similar to the routine powder diffraction technique, single crystal diffraction can provide structure-related information about the sample, including lattice parameters, density and equation of states. On the other hand, more knowledge beyond crystal structure can be extracted from single crystal diffraction, such as chemical bonding, anisotropy and lattice dynamics. Single crystal diffraction requires careful sample preparation, sophisticated instrumentation and advanced data analysis software, which increases its entrance barrier in comparison with the straightforward powder diffraction. Though most Earth related materials have been thoroughly studied with powder diffraction, many major components in the mantle and core haven't been systematically measured by single crystal diffraction yet.

As stated above, Partnership for eXtreme Xtallography (PX^2) is providing new capabilities for high-pressure diamond anvil cell research at the GSECARS APS beamline. The PX^2 project is a collaboration between the University of Hawaii and GSECARS. Supported by COMPRES and hosted by GSECARS at experimental station 13-BM-C. PX^2 started general user support from February 2015, and more than 80% of our users are from COMPRES member institutions. Different from most synchrotron beamlines that carry out powder diffraction experiments, the PX^2 beamline features a focused, monochromatic 29 keV incident beam and a unique 6-circle heavy duty Newport diffractometer, optimized for variety of advanced crystallography experiments, including interface studies, powder and single crystal structure determination, equation of state studies and diffuse scattering analysis. Through this one day training event, we hope to attract more users, especially young scientists, in the COMPRES community to collaborate with PX^2. We would also like to inspire collaboration between crystallographers and experts of other high pressure related techniques.

#### **Activities**:

- Plenary session: single-crystal X-ray diffraction in multidisciplinary extreme condition science
- Instruction session: sample preparation, data collection and data analysis
- Hands-on exercises: demonstrations various aspects of data collection and analysis

**Desired outcomes**: Advertise the PX^2 facility to the international high pressure community and new COMPRES users. Inspire new crystallography related research collaborations between the PX^2 facility and other institutions. Educate young scientists about the basic principles of single crystal sample preparation, data collecting and analysis. We intend to attract students and early-career scientists, preferably those who are interested but do not have extensive prior experience about single crystal diffraction. We will encourage attendees to bring their own sample, and we plan to reserve one day of time at the in house XRD lab in Hawaii after the workshop for interested attendees to collect single crystal data on their own samples. The training event will take place on campus of the University of Hawaii. Participation in the training event will be offered to IUCr HP workshop participants at no extra cost, but because of the computer lab space limits, will be restricted to 20 students. We expect 5 experienced instructors, including beamline scientists from two COMPRES beamlines to participate in the training event.

## Przemyslaw Dera, Ph.D.

Hawaii Institute of Geophysics and Planetology • School of Ocean and Earth Science and Technology • University of Hawaii at Manoa 1680 East West Road (POST Bldg) • Honolulu, Hawaii 96822 Tel. (630) 252-0419 • Fax (630) 252-0436 • E-mail pdera@hawaii.edu

#### A. PROFESSIONAL PREPARATION

Adam Mickiewicz University, Poznan, Poland

M.Sc. in theoretical chemistry (Summa Cum Laude) 1995

Adam Mickiewicz University, Poznan, Poland

Ph.D. in physical and theoretical chemistry 2000

#### **B.** APPOINTMENTS

## Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa

2016/8- R5 Researcher (Full Professor) tenured

2013/8-2016/7 R4 Associate Researcher (Assoc. Professor) tenure track

### Department of Geology, University of Illinois at Urbana-Champaign

2011-2013 Adjunct Associate Professor

### Consortium for Advanced Radiation Sources, The University of Chicago

2013- Visiting Scholar

2010-2013 Senior Research Associate (tenured)

2007-2010 Research Beamline Scientist (tenure track)

## Geophysical Laboratory, CIW

2003-2007 Associate Staff Scientist (principal investigator)

2002-2003 Senior Research Scientist

2000-2002 Distinguished Barbara McClintock Postdoctoral Fellow

1998 Predoctoral Fellow

#### **C. PRODUCTS**

#### Most relevant products

- Lavina B., <u>Dera P.</u> and Downs R.T. "Modern X-ray Diffraction Methods in Mineralogy and Geosciences" (2014) Reviews in Mineralogy & Geochemistry, Mineralogical Society of America, Vol. 78, pp. 1-31.
- Dera P., Zhuravlev K., Prakapenka V., Rivers M.L., Finkelstein G.J., Grubor-Urosevic O., Tschauner O. Clark S.M. and Downs R.T. "High-pressure single-crystal micro- X-ray diffraction (SCμXRD) analysis with GSE\_ADA/RSV software" (2013) High Pressure Research 33, 466-484.
- Plonka A., <u>Dera P.</u>, Irmen P., Rivers M.L., Ehm L., and Parise J.B. "β-diopside, a new ultrahigh-pressure polymorph of CaMgSi<sub>2</sub>O<sub>6</sub> with six-coordinated silicon" (2012) Geophys. Res Letters **39**, L24307.
- Dera P. and Weidner D. (Eds) "Mineral Physics Harnessing the Extremes: From Atoms and Bonds to Earthquakes and Plate Tectonics. 2016 Long-Range Planning Report" (2016) GeoProse.
- Lavina B., <u>Dera P.</u>, Kim E., Meng Y., Downs R.T., Weck P.F., Sutton S.R. and Zhao Y. "Fe<sub>4</sub>O<sub>5</sub>, a new, recoverable, high pressure-temperature iron oxide" (2011) Proc. Natl. Acad. Sci. **108**, 17281-17285.

#### Other significant products

- El Goresy A., <u>Dera P.</u>, Sharp T.G., Prewitt C.T., Chen M., Dubrovinsky L., Wopenka B., Boctor N.Z., Hemley R.J. "Seifertite, a dense orthorhombic polymorph of silica from the Martian meteorites Shergotty and Zagami" Euro. J. Mineral. (2008) **20**, 523-528.
- Zhang L., Meng Y., <u>Dera P.</u>, Yang W., Mao W.L., Mao H.-K. "Single-crystal structure determination of (Mg,Fe)SiO<sub>3</sub> postperovskite" (2013) Proceedings of the National Academy of United States doi: 10.1073/pnas.1304402110.
- Jacobsen S.D., Holl C., Adams K., Fischer R., Martin E., Bina C., Lin J.F., Prakapenka V.B., Kubo A., <u>Dera P.</u> "Compression of single-crystal magnesium oxide to 118 GPa and a ruby pressure gauge for helium pressure media" American Mineralogist (2008) **93**, doi: 10.2138/am.2008.2988.
- <u>Dera P.</u>, Lavina B., Borkowski L.A., Prakapenka V.B., Sutton S., Rivers M.L., Downs R.T., Boctor N.Z., Prewitt C.T. "High-pressure behavior and structure barringerite Ni-end member Ni<sub>2</sub>P and its implications for phosphide phases in planetary cores" Journal of Geophys. Res. **114** (2009) B03201.
- <u>Dera P.</u>, Lazarz J., Prakapenka V.B., Barkley M., Downs R.T. "New insights into high-pressure polymorphism of SiO<sub>2</sub> cristobalite" Physics and Chemistry of Minerals (2011) **38**, 517-529.

## **D. SYNERGISTIC ACTIVITIES**

- COMPRES Distinguished Lecture Series (2014-2015).
- Elected Fellow, Mineralogical Society of America (2013).
- Chair of the International Union of Crystallography Commission on High Pressure (2008-2014).
- Member (2010-2012) and Vice Chair (2012-2013) of Executive Committee, Consortium for Materials Properties Research in Earth Science (COMPRES)
- Book Editor "High-pressure Crystallography" published by Springer Science for Peace and Security Series B.

## **Dongzhou Zhang**

Partnership for Extreme Crystallography, University of Hawaii at Manoa, 9700 S. Cass Ave, Bldg 434A, Argonne, IL 60439 Tel: 630-252-0444, Email: dzhang@hawaii.edu

## A. Professional preparation

Peking University, Beijing, China,	B.Sc. in Physics,	2008
California Institute of Technology, Pasadena, CA, USA,	M.Sc. in Geophysics,	2010
California Institute of Technology, Pasadena, CA, USA,	Ph.D. in Geophysics,	2015

#### **B.** Appointments

#### Partnership for Extreme Crystallography, University of Hawaii at Manoa

2015/1- Beamline Scientist

# Hawaii Institute of Geophysics and Planetology, University of Hawaii at Manoa 2015/9- Adjunct Researcher

### Advanced Photon Source, Argonne National Laboratory

2012-2014 Laboratory Graduate Appointment

#### C. Products

### *Most relevant products*

- Zhang, D., Jackson, J.M., Zhao, J., Sturhahn, W., Alp, E.E., Hu, M.Y., Toellner, T.S., Murphy, C.A., and Prakapenka, V.B. (2016) Temperature of Earth's core constrained from melting of Fe and Fe<sub>0.9</sub>Ni<sub>0.1</sub> at high pressures. Earth and Planetary Science Letters, *447*, 72-83
- Zhang, D., Jackson, J.M., Zhao, J., Sturhahn, W., Alp, E.E., Toellner, T.S. and Hu, M.Y. (2015) Fast temperature spectrometer for samples under extreme conditions. Review of Scientific Instruments, *86*, 013105.
- Chen, B., Li, Z., Zhang, D., Liu, J., Hu, M.Y., Zhao, J., Bi, W., Alp, E.E., Xiao, Y., Chow, P. and Li, J. (2014) Shear softening in low-spin Fe<sub>7</sub>C<sub>3</sub> and implications for the solidity of Earth's inner core, Proceedings of the National Academy of Sciences, *111*(50), 17755-17758.
- Zhang, D., Jackson, J.M., Chen, B., Sturhahn, W., Zhao, J., Yan, J., and Caracas, R. (2013) Elasticity and lattice dynamics of enstatite at high pressure, Journal of Geophysical Research-Solid Earth, *118*, B50303.
- Chen, B., Jackson, J.M., Sturhahn, W., <u>Zhang, D.</u>, Zhao, J., Wicks, J.K., and Murphy, C.A., (2012) Spin crossover equation of state and sound velocities of (Mg<sub>0.65</sub>Fe<sub>0.35</sub>)O ferropericlase up to 140 GPa, Journal of Geophysical Research-Solid Earth, *117*, B08208.

#### Other significant products

- Chen, T., Akciz, S.O., Hudnut, K.W., <u>Zhang, D.</u> and Stock, J.M. (2015) Fault-slip distribution of the 1999 Mw 7.1 Hector Mine earthquake, California, estimated from postearthquake airborne LiDAR data, Bulletin of the Seismological Society of America, *105*, 776-790.
- Zhang, D., Jackson, J.M., Sturhahn, W., and Xiao, Y. (2011) Local structure variations observed in orthoenstatite at high-pressures, American Mineralogist, *96*, 1585-1592.
- Chen, Z.L., Li, Y., Liu, W.W., <u>Zhang, D.</u>, Zhao, Y.Y., Yuan, B., and Jiang, X.Y. (2009) Patterning Mammalian Cells for Modeling Three Types of Naturally Occurring Cell-Cell Interactions. Angewandte Chemie-International Edition *48*, 8303-8305.
- Yang, D.Y., Wang, Y., Zhang, D., Liu, Y.Y., and Jiang, X.Y. (2009) Control of the

morphology of micro/nanostructures of polycarbonate via electrospinning. Chinese Science Bulletin *54*, 2911-2917.

Jiang, X., Yang, D., <u>Zhang, D.</u> and Jiang, J. (2008) Apparatus for preparing macromolecule nanofibre and spinning method thereof, Chinese Patent CN101314869.

## **D.** Synergistic Activities

- Major Partner: Advanced Photon Source Partner User Proposal: Novel fast temperature measurements for nuclear resonant scattering experiments under extreme conditions. Development of new research tools in a national user facility.
- Reviewer for American Mineralogist, since 2010.
- Developer of data collection/analysis software suite at the Advanced Photon Source: FasTeRRead, FasTeRSim and FasTeRCali, since 2013.
- Instructor of single crystal diffraction data analysis for the users of the Advanced Photon Source, since 2015.
- American Geophysical Union Mineral and Rock Physics Graduate Research Award, 2015.

SUMMARY YEAR 1
PROPOSAL BUDGET FOR NSF USE ONLY

ORGANIZATION			PROPOSAL NO. DURATION			
University of Hawaii				Proposed		Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR		A	WARD N	0.		
Przemyslaw Dera						
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associates	s	NSF Fund Person-mo	ded nths		unds ested By	Funds granted by NSF
(List each separately with title, A.7. show number in brackets)	CAI	ACAD	SUMR	pro	poser	(if different)
1.	0.0	0.00	0.00	,		
2.						
3.						
4.						
5.						
6. ( 0) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAG	E) 0.0	0.00	0.00			
7. ( 1) TOTAL SENIOR PERSONNEL (1 - 6)	0.0	0.00	0.00		0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. ( <b>0</b> ) POST DOCTORAL SCHOLARS	0.0	0.00	0.00		0	
2. ( <b>0</b> ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.0	0.00	0.00		0	
3. ( <b>0</b> ) GRADUATE STUDENTS					0	
4. ( <b>0</b> ) UNDERGRADUATE STUDENTS					0	
5. ( <b>0</b> ) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0	
6. ( <b>0</b> ) OTHER					0	
TOTAL SALARIES AND WAGES (A + B)					0	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					0	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					0	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCEI	EDING \$5	5,000.)				
·		•				
TOTAL EQUIPMENT					0	
E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)					0	
2. INTERNATIONAL					Ö	
F. PARTICIPANT SUPPORT COSTS						
1. STIPENDS \$						
2. TRAVEL 5,000						
3. SUBSISTENCE						
4. OTHER 5,000						
TOTAL NUMBER OF PARTICIPANTS ( 0) TOTAL PA	RTICIPA	NT COST	S		10,000	
G. OTHER DIRECT COSTS	arrion /	111 0001	<u> </u>		10,000	
					0	
1. MATERIALS AND SUPPLIES 2. PURPLICATION COSTS/DOCUMENTATION/DISSEMINATION						
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION  2. CONSULTANT SERVICES						
3. CONSULTANT SERVICES						
4. COMPUTER SERVICES						
5. SUBAWARDS					0	
6. OTHER						
TOTAL OTHER DIRECT COSTS (A TURQUICUS)						
H. TOTAL DIRECT COSTS (A THROUGH G)					10,000	
I. INDIRECT COSTS (F&A)(SPECIFY RATE AND BASE)						
(Rate: , Base: )						
TOTAL INDIRECT COSTS (F&A)					0	
J. TOTAL DIRECT AND INDIRECT COSTS (H + I)					10,000	
K. SMALL BUSINESS FEE					0	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)					10,000	
M. COST SHARING PROPOSED LEVEL \$ <b>0</b> AGREED LEVEL IF DIFFERENT \$						
				E ONLY		
Przemyslaw Dera					E VERIFIC	
ORG. REP. NAME*		Date Checke	d Dat	e Of Rate	Sheet	Initials - ORG

SUMMARY Cumulative
PROPOSAL BUDGET FOR NSF USE ONLY

ORGANIZATION			OPOSAL	NO.	DURATIO	ON (months)
University of Hawaii				Proposed		Granted
PRINCIPAL INVESTIGATOR / PROJECT DIRECTOR	A'	WARD N	Ο.			
Przemyslaw Dera						
A. SENIOR PERSONNEL: PI/PD, Co-PI's, Faculty and Other Senior Associate	1 crock monato			Regu	unds Lested By	Funds granted by NSF
(List each separately with title, A.7. show number in brackets)	CAI	_ ACAD	SUMR	pro	oposer	(if different)
1.	0.0	0.00	0.00			
2.	$\perp$					
3.	$\perp$			<u> </u>		
4.				<u> </u>		
5.						
6. ( ) OTHERS (LIST INDIVIDUALLY ON BUDGET JUSTIFICATION PAG					0	
7. ( <b>0</b> ) TOTAL SENIOR PERSONNEL (1 - 6)	0.0	0.00	0.00		0	
B. OTHER PERSONNEL (SHOW NUMBERS IN BRACKETS)						
1. ( <b>0</b> ) POST DOCTORAL SCHOLARS	0.0				0	
2. ( <b>0</b> ) OTHER PROFESSIONALS (TECHNICIAN, PROGRAMMER, ETC.)	0.0	0.00	0.00		0	
3. ( <b>0</b> ) GRADUATE STUDENTS					0	
4. ( <b>0</b> ) UNDERGRADUATE STUDENTS					0	
5. ( 0) SECRETARIAL - CLERICAL (IF CHARGED DIRECTLY)					0	
6. ( <b>0</b> ) OTHER					0	
TOTAL SALARIES AND WAGES (A + B)					0	
C. FRINGE BENEFITS (IF CHARGED AS DIRECT COSTS)					0	
TOTAL SALARIES, WAGES AND FRINGE BENEFITS (A + B + C)					0	
D. EQUIPMENT (LIST ITEM AND DOLLAR AMOUNT FOR EACH ITEM EXCE	EDING \$5	,000.)				
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E. TRAVEL 1. DOMESTIC (INCL. U.S. POSSESSIONS)					0	
2. INTERNATIONAL					0	
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F. PARTICIPANT SUPPORT COSTS  1. STIPENDS \$						
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2. IRAVEL <b>O</b>						
3. SUBSISTENCE 5,000						
4. OTHER	NDTICIDA	NT COST			10 000	
G. OTHER DIRECT COSTS	KIICIPA	.N1 COS1	5		10,000	
1. MATERIALS AND SUPPLIES					0	
					0	
2. PUBLICATION COSTS/DOCUMENTATION/DISSEMINATION						
3. CONSULTANT SERVICES						
4. COMPUTER SERVICES						
5. SUBAWARDS					0	
6. OTHER						
TOTAL OTHER DIRECT COSTS  H. TOTAL DIRECT COSTS (A THROUGH G)					0 10,000	
					10,000	
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TOTAL INDIRECT COSTS (F&A)  J. TOTAL DIRECT AND INDIRECT COSTS (H + I)					0 10,000	
TOTAL DIRECT AND INDIRECT COSTS (H + I)  K. SMALL BUSINESS FEE					10,000 N	
					10,000	
L. AMOUNT OF THIS REQUEST (J) OR (J MINUS K)					10,000	
M. COST SHARING PROPOSED LEVEL \$ 0 AGREED LEVEL IF DIFFERENT \$				UCE III	T ONLY	
PI/PD NAME	ŀ	INIDID			SE ONLY	DATION
Przemyslaw Dera  ORG, REP. NAME*		INDIKI Date Checked		e Of Rate	E VERIFIC	Initials - ORG
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**Budget Justification** 

F. Participant Support Costs

This proposal requests funds for 10 young scientist travel awards to enable participation of

graduate students, postdoctoral researchers and young tenure-track faculty in the 2018 Workshop of the International Union of Crystallography Commission on High Pressure in

Honolulu, HI.

The travel awards will be granted at \$1,000/person and will cover registration fee (\$6000)

regular participant, \$400 student) and portion of the travel expenses. The travel awards will be

limited to participants affiliated with research or academic institutions in the USA.

H. Total Direct Costs \$10,000

I. Indirect Costs: No indirect costs are applied, as the only budget category requested is Participant

Support.

J. Total Direct and Indirect Costs: \$10,000

L. Amount of this Request: \$10,000

## **Current and pending support**

#### Current and Pending Support, Przemyslaw K Dera Title of Award Point of Contact & Phone Period of Budget (\$K) & Sponsoring Institution or Project & Email Performance Commitment (WY) **CURRENT SUPPORT: COMPRES** \$916,728 Partnership for Extreme subcontract (NSF Xtallography and 10% effort Carl Agee EAR IF) under NSF 06/01/2014 to COMPRES Technology Role: PI agee@unm.edu Cooperative 05/31/2018 Office - Operation No salary support Agreement EAR 11-57758 for the PI \$559.701 (UH subcontract Integration of Synchrotron NSF Software Thomas F. Russell, budget \$41,577) X-ray Analysis Software Infrastructure for 09/01/2015 to trussell@nsf.gov Methods into the Larch 08/31/2018 Sustained 5% effort Framework (#1450468) Innovation 1 month salary in year 3 Development of X-ray Atlas, a high-brilliance \$599,994 high-sensitivity high-load-Russell Kelz 10% effort capacity X-ray **NSF EAR** rkelz@nsf.gov 04/15/2016 to diffractometer for Instrumentation Role: PI 3/31/2019 mineralogy and mineral and Facilities 1 month salary physics research at the in years 2 and 3. University of Hawaii (#1541516) \$360,000 10% effort, 1 Robin Reichlin Fate and role of month salary in rreichli@nsf.gov NSF EAR 06/01/2017 to metastable pyroxenes in years 2 and 3. Geophysics 5/31/2020 the subduction process Role: PI Support for the CheMin \$34,000 mineralogical instrument 5% effort. 1 during the Mars Science Robert Downs 06/01/2017 to person/months in NASA Laboratory 5/31/2019 rdowns@email.arizona.edu years 1 and 2. 2017-2019 extended mission 2

## Przemyslaw K Dera, University of Hawaii at Manoa

Status: Pending (proposed duration 09/01/2018-8/31/2023)

NSF NRT, \$2,999,430

"NRT: Innovative Materials and Technologies for an Adaptable Future (IMTAF)"

PI: P. Dera

Commitment: 1 months in years 1-5

Status: Pending (proposed duration 08/01/2018-07/31/2023)

NSF EAR Instrumentation and Facilities, \$712,178

"Laboratory Technician Support: Experimental Mineral Physics and Petrology Facilities at the University of Hawaii at Manoa"

PI B. Chen (University of Hawaii)

Commitment: 10% effort, no salary support for Dera

Status: Pending (proposed duration 11/01/2018-10/29/2021)

NASA SSW, \$166,720

"The petrogenesis of poorly crystalline martian mudstone: Use of a basaltic catchment basin in Hawaii as a terrestrial analog"

PI: T. Bristow (NASA Ames),

Commitment: 5% effort, month in years 2 and 3.

Status: Pending/This proposal (proposed duration 07/01/2018-12/31/2018)

NSF EAR Geophysics, \$10,000

"Support for 2018 IUCr High Pressure Workshop in Honolulu, HI"

PI: P. Dera (University of Hawaii)

Commitment: 2% effort, no salary support for Dera

# **Current and pending support**

Dongzhou Zhang, University of Hawaii at Manoa

Status: Pending/This proposal (proposed duration 07/01/2018-12/31/2018)

NSF EAR Geophysics, \$10,000

"Support for 2018 IUCr High Pressure Workshop in Honolulu, HI"

PI: P. Dera (University of Hawaii) Commitment: 2% effort, no salary support