Application for a Humboldt Research Fellowship in Germany for applicants from abroad



Please complete the form online. You can save data at any time and send the completed form online to the Humboldt Foundation.

For the time being, **researchers from Brazil** can only apply for a Capes-Humboldt Research Fellowship. Thus applications using this form can unfortunately not be processed.

Academics from developing and transition countries may be eligible to apply for a Georg Forster Research Fellowship.

Family name	Messerly
First name(s) / Given name(s)	Richard

Application for a

•	Humboldt Research Fellowship for postdoctoral researchers ¹ (Programme information (PDF) / FAQ)
C	Humboldt Research Fellowship for experienced researchers ² (Programme information (PDF) / FAQ)

 $^{^{1}}$ The term postdoctoral refers to highly-qualified researchers at the beginning of their academic careers who completed their doctorates less than four years ago.

 $^{^2}$ Experienced researchers are highly-qualified academics with a clearly defined academic profile who completed their doctorates less than twelve years ago.

1. Personal details

Title	Dr.
Family name	Messerly
First name(s) / Given name(s)	Richard
Former family name	
Date of birth	21.06.1987
Gender	⊙ male C female
Nationality	United States of America
Additional nationality	
Present professional position	NRC Postdoc
Highest academic degree	PhD
Email address	r.alma.messerly@gmail.com edit

2. Institution at which you are currently working

Country	United States of America		
City / Town	Boulder Postal code Colorado		
University/Institution	National Institute of Standards and Technology		
Department / Institute	Thermodynamics Research Center		
Street, P.O. Box	325 Broadway		
Phone number	1 303 4973295		

3. **Private address** – only if contact address

Country	United States of America		
City/Town	Superior	Postal code	Colorado
Street, P.O. Box	1995 E Coalton Rd. 89-102		
Phone number	1 801 3581741		

4. Indicate the address to which correspondence should be

C Address of the institute	Private address

5. Last institution outside Germany, if you are already working in Germany

Country		
City / Town	Postal code	
University/Institution		
Department / Institute		
Street, P.O. Box		

6. Host and host institute

Title	Dr.		
Family name	Vrabec		
First name(s)	Jadran		
Country	Germany		
City/Town	Berlin Postal code Berlin		
University/Institution	Technische Universitat Berlin		
Department / Institute	Institut für Prozess- und Verfahrenstechnik		
Street, P.O. Box	Straße des 17. Juni 135, 10623		
Phone number	49 30 31422646		
Faxnumber	49 30 31422406		
Email address	vrabec@tu-berlin.de		

Ask your host to upload their review and confirmation of research facilities.

Request documents

Host's statement	Afile was uploaded on 10.07.2018.
Host's confirmation of research facilities	Afile was uploaded on 10.07.2018.

7. **Second host** and **host institute** if you intend to conduct your research with two hosts

Title		
Familyname		
First name(s)		
Country	Germany	
City/Town		Postal code
University/Institution		
Department / Institute		
Street, P.O. Box		
Phone number		
Faxnumber		
Email address		

Ask your host to upload their review and confirmation of research facilities.

Request documents

Host's statement	No file has been uploaded yet.
Host's confirmation of research facilities	No file has been uploaded yet.

7a. **Scheduled period** and number of months **to be spent at the second host institute** if the research work is to be carried out at two host institutes

Starting date		Number of months	
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7b. I plan to spend part of my research stay – 25 per cent max of the estimated sponsorship period – in a different European country (not my country of origin).

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-		-	
(C)	Vac	(•)	No
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Curriculum vitae

8. **Academic / Professional record** in reverse chronological order (starting with your current position and going back to your first university degree), including career breaks

Please provide a seamless overview of every stage of your career according to this example (PDF). This CV plays an important role in reviewing your application, so please include all relevant information.

From	То	Position	Institution, City	Country	Degrees / Remarks ³
02.2017	today	Postdoc Associate	National Institute of Standards and Technology, Boulder	United States of America	100% research; National Research Council Associateship
01.2012	04.2017	Doctoral student	Brigham Young University, Provo	United States of America	Doctorate in Chemical Engineering
01.2012	02.2014	Research Assistant	Design Institute for Physical Properties, Provo	United States of America	Part time (50%)
01.2012	04.2012	Teaching Assistant	Brigham Young University, Provo	United States of America	Part time (50%)
07.2010	12.2011	Research Assistant	Brigham Young University, Provo	United States of America	Part time (50%)
12.2008	12.2012	Student	Brigham Young University, Provo	United States of America	Bachelor of Science in Chemical Engineering
11.2006	11.2008	No position	Church of Jesus Christ of Latter- day Saints, Quetzaltenango	Guatemala	Religious Service Mission (LDS)
08.2005	11.2006	Student	Brigham Young University, Provo	United States of America	Bachelor of Science in Chemical Engineering

³ Examples: Type of university degree (title as used in your country) and field of study/research / if you received a fellowship, provide name of the funding body / time dedicated to research in per cent / reasons for interrupting your career (e.g. parental leave, military service, severe illness) / in case of parental leave, state child's date of birth and percentage of scientific work conducted during this period, if relevant.

8a. For experienced researchers: Please give the names of the doctoral candidates you have already supervised:

Family name	First name(s) / Given name(s)

Academic profile and fellowship period

9. Field of research

Research area	Organic Molecular Chemistry	Code of research area	F10201
Second research area if applicable		Code of research area	

10. Details of doctoral thesis and doctoral degree

Title of thesis (for Ph.D, C.Sc, etc.)	How Uncertainty Quantification Quantitative Tool for predicting	Renders Molecular Simulation a thermophysical properties	
Date of doctoral degree	07.12.2016	Grade obtained if applicable	

11. Are you currently **preparing for an academic examination** or degree (e. g. Ph.D.)?

•	No		
C	Yes		
	Country		
	City/Town		
	Name of institution		
	Expected date	Degree	
	Major subject studied / examined		

12. Proposed fellowship period at the host institute

Postdoctoral researchers (6-24 months)

Starting date 02.2019 Number of months 24

Experienced researchers (6-18 months)

Period 1		Period 2		Period 3	
Starting date		Starting date		Starting date	
Number of months		Number of months		Number of months	

Total number of months	

13. Short abstract of your research proposal

Title of research proposal (200 characters max)

Advancing the hybrid data set approach towards reliable mixture properties: Going beyond the traditional Lennard-Jones potential

Keywords (up to five) to define your particular research topic a	at the host institute	
Molecular simulation (Monte Carlo/Molecular dynamics)	Equation of state	Force field development
Thermophysical Properties	Non-bonded potentials	

Brief summary (2,000 characters max) of the research proposal (please upload detailed description under No.26)

Reliable estimates of thermophysical properties are essential for designing efficient and reliable technical processes. Fundamental equations of state (FEOS) based on the Helmholtz energy allow for prediction of pressure, density, temperature behavior as well as energetic properties, e.g., heat capacities. Unfortunately, most pure species (and, to a greater extent, mixtures) do not have enough reliable experimental data to fit the large number of FEOS parameters. In this case, molecular simulation can supplement experimental data at state points where reliable data are scarce, typically at high temperatures and pressures.

The primary limitation of this so-called "hybrid data set" approach is the accuracy of the force field used in the molecular simulation. Specifically, most force fields perform well for vapor-liquid equilibrium properties but extrapolate poorly to high pressures. As thermophysical properties are highly sensitive to the non-bonded interactions, we propose using the extended Lennard-Jones (ex-LJ) potential, which is significantly more flexible than the traditional Lennard-Jones 12-6 potential. Furthermore, we propose an iterative hybrid data set approach, where the ex-LJ parameters are reoptimized after each iteration to ensure self-consistency between the FEOS and the force field.

To reduce the computational cost of this iterative approach, we will implement Multistate Bennett Acceptance Ratio (MBAR) combined with basis functions. In my previous work, I demonstrated that MBAR with basis functions yields extremely fast and reliable estimates of thermophysical property values for any force field parameter set, without performing direct molecular simulation. My expertise with MBAR and basis functions combined with the host's simulation infrastructure and hybrid data set approach makes this an ideal pairing. Furthermore, as we both collaborate closely with expert FEOS developers, the success of this project is very promising.

13a. What do you think will be the **impact** of your research on the **further development of your own academic profile**? (2000 characters max)

I intend on making the proposed methodology, "iterative hybrid data sets," the keystone of my future research. During a two-year postdoc, it would be impossible to develop equations of state and force fields for every compound of interest. I will continue to implement this approach for years to come with additional molecular species/mixtures.

My long-term career path is to become a professor, but with a strong emphasis on "industrially relevant" research. The proposed research is exemplary of this as it utilizes state-of-the-art scientific/academic methods but with the ultimate impact found in industry. An important benefit of this research is that it allows me to pursue a career path in academia, industry, or a government agency.

In brief, there are four key facets in which the proposed research will significantly impact the development of my academic profile:

- 1) Expertise/skills
- 2) Leadership
- 3) Diversification
- 4) Networking

Working with Vrabec, a pioneer in hybrid data sets, will greatly accelerate and deepen my understanding of this approach. Furthermore, I will explore the details and better appreciate the challenges of fitting equations of state with high-dimensional non-linear models. This skill will be invaluable throughout my career, regardless of the path I pursue. Since I will contribute to the molecular simulation package developed by Vrabec's group, ms2, I will learn Fortran 90, a valuable coding language. By working directly with the developers of ms2, I will be equipped to participate more in future code development.

As my previous research groups were relatively small, joining Vrabec's group is a great opportunity for me to see firsthand how larger research groups function. Mentoring undergraduates and doctoral candidates will improve my leadership and teaching skills. Under Vrabec's tutelage, I will develop my own teaching style and research plan. I will greatly benefit from the diversity and global network found at a German university.

Applicant's language proficiency

14. Knowledge of languages

Assess your proficiency in reading, writing, listening comprehension and speaking according to the Common European Framework of Reference for Languages in the following languages.

C2 Proficiency/ First language C1 Advanced B2 Upper intermediate B1 Intermediate A2 Elementary A1 Beginner None

		Reading	Writing	Listening	Speaking
English		C2	C2	C2	C2
German		none	none	none	none
Others	Spanish	C1	B2	B2	B2
	French	B2	B1	B1	B1
	Portuguese	B2	A2	B1	A2

15. German language courses attended

			,		
Fr	om	То	1	Name of language school	City/Town
Have	Have you taken a German language examination?				
C	Yes	6	No		
If so, which, when and where?					

16. Grant for an intensive German language course

fello	wship? Participation in su ediately prior to the resea	uch co arch s	ourses is recommended. tay, this means that you v	. Intens	uage course before starting the research sive language courses in Germany take place y begin your research work at the host institute rse does not count towards the fellowship period.
C	C Yes (2 months) C Yes (4 months) C No				
	If possible, starting on				

⊙	No	0	Yes		
		lf s	o, in what y	ear?	
8. A	re you ap	plying to	any oth	ner ins	stitution for a fellowship?
•	No	O	Yes		
		If so, to w	hich institut	tion?	
also		you apply fo			made on any application you have made to other institutions. Please ny other institutions after having submitted your application to the
luml					g simultaneously for funding from the Alexander von ently receiving funding from the Alexander von Humbolo
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⊚	No	0	Yes		
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21. Names and addresses of **expert reviewers**

Title	Dr.
Family name	Wilding
First name(s)	Vince
Doctoral supervisor	© Yes C No
Country	United States of America
City/Town	Provo
University/Institution	Brigham Young University
Email address	vincent_wilding@byu.edu

Please ask your expert reviewer to upload his or her review.

Request review

Expert review	Afile was uploaded on 06.07.2018.
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Title	Dr.
Family name	Hasse
First name(s)	Hans
Country	Germany
City/Town	Kaiserslautern
University/Institution	Technical University of Kaiserslautern
Email address	hans.hasse@mv.uni-kl.de

Please ask your expert reviewer to upload his or her review.

Request review

Expert review	Afile was uploaded on 07.07.2018.
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Declarations

22. Declaration of Commitment

Please check the box, otherwise it will not be possible to process your application.

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I hereby declare that the above statements are correct and complete and that I am not aware of any health issues that would impede my ability to complete the planned research stay.

I confirm that I have taken note of the Alexander von Humboldt Foundation's Rules of Good Scientific Practice and agree to the regulations set out therein. I further confirm that I have adhered to the rules of good scientific practice in my scientific work to date.

Furthermore, I declare that neither in my academic work to date nor in conducting the research proposed in this application have I contravened or will contravene the legally-binding principles of scientific ethics. Moreover, I confirm that there is no danger of armaments-related technology transfer as defined by statutory regulations.

In the Guidelines and Information for Research Fellows you will find information on the Rules of Good Scientific Practice, statutory regulations and general obligations.

Date of application: 10.07.2018

23. Declaration of consent to funding through collaborative partnerships

Please check one of the radiobuttons, otherwise it will not be possible to process your application.

In the event of a positive decision on my application I would also be interested in sponsorship through a collaborative partner of the Alexander von Humboldt Foundation. Information on current collaborative partners in the Humboldt Research Fellowship Programme can be found on our website.

I further agree that in the event of a positive decision the Alexander von Humboldt Foundation may forward my application documents with my personal information and details of my intended research stay in Germany to the collaborative partners selected by the Foundation.

Date of application: 10.07.2018

©	V	0	NI-
100	Yes	5-2	No

24. Data Privacy Statement

Please check the box, otherwise it will not be possible to process your application.

⊽

I hereby agree to the Alexander von Humboldt Foundation storing the information I provided upon submission of my application and using this data to process my application.

I furthermore consent to the Alexander von Humboldt Foundation electronically storing and processing data relating to my person (surname, first name, academic title, field of research and specialism, country, gender, postal address, e-mail address, current or last university/institution, date of birth, career details, and, where applicable, first sponsorship through the Humboldt Foundation) upon my submission of the application and to the use of this data for purposes of review, statistics and evaluation by the Alexander von Humboldt Foundation and its authorised agents in accordance with Article 28 of the General Data Protection Regulation (GDPR); the results of the evaluation will be published only in a cumulative, anonymised form.

I hereby agree to the Alexander von Humboldt Foundation, in the event that my application is approved, publishing this information, stating my name, academic title, field of research and specialism, country and career details.

I hereby agree to my data being stored for a period of three years for the above-mentioned purposes as well as to facilitate the submission of later applications, and to it being subsequently anonymised. This period begins with the date on which the Humboldt Foundation issues a negative decision on the application. The data will be stored on servers belonging to the Humboldt Foundation or, in the case of processing on behalf of the controller, on the processor's servers; personal data will not be transferred to third parties as defined by Article 4 (10) of the General Data Protection Regulation (GDPR).

I have also been informed that my consent to the collection, processing and use of my data is voluntary and that I may revoke my consent at any time for the future. Where applicable, I will send my revocation to info@avh.de. In the event that I revoke my consent while my application is still being processed, my data will be erased. Should I revoke my consent after my rejected application has been processed, my data will be anonymised.

Data protection officer of the Alexander von Humboldt Foundation: ansgar.schuldenzucker@avh.de Date of application: 10.07.2018

Additional personal details

25. Additional personal details

Below we should like to ask for some additional, personal details (optional). If your application is approved, they will enable the Alexander von Humboldt Foundation to send you the award documents as soon as possible. In addition, they will be used to create the necessary conditions to take decisions on applications for a subsidy towards health insurance, family allowances and grants for German language courses as well as to budget the necessary financial resources in advance. If you are not awarded a Humboldt Research Fellowship, the following data will not be stored electronically. These data are not relevant to the Selection Committee's decision and will not be presented to the Committee.

Applicant's country of birth	United States of America		
Applicant's place of birth	Eureka, California		
Marital status	married		
Family name of marital partner	Migliori		
First name(s) of marital partner	Erica		
Children's dates of birth – only if n	ot completed under No. 8 (dd.mm.yyyy)		
25.07.2013 20.08.2015			

26. Required additional application documents

All application documents must be uploaded in German or English.

Please upload the additional documents that are required for your application here. Please note that we can only accept documents in PDF format without any write, read or print protection (maximum file size per document: 10 MB).				
Curriculum vitae (two pages max) Curriculum_Vitae_Humboldt.pdf	Research outline (five pages max) Humboldt_rough_draft.pdf			
Complete list of publications List_publications_Humboldt.pdf	List of selected key publications Key_publications_Humboldt.pdf			
Publishers' letter(s) of acceptance	Publishers' acknowledgment(s) of receipt 1_submitted_manuscript.pdf 2_submitted_manuscript.pdf			
Key publications 1_key_publication.pdf 2_key_publication.pdf 3_key_publication.pdf	Summaries / Translations			
Doctoral certificate Messerly_eDiploma.pdf Messerly_Electronic_Transcript.pdf	German language certificate			