



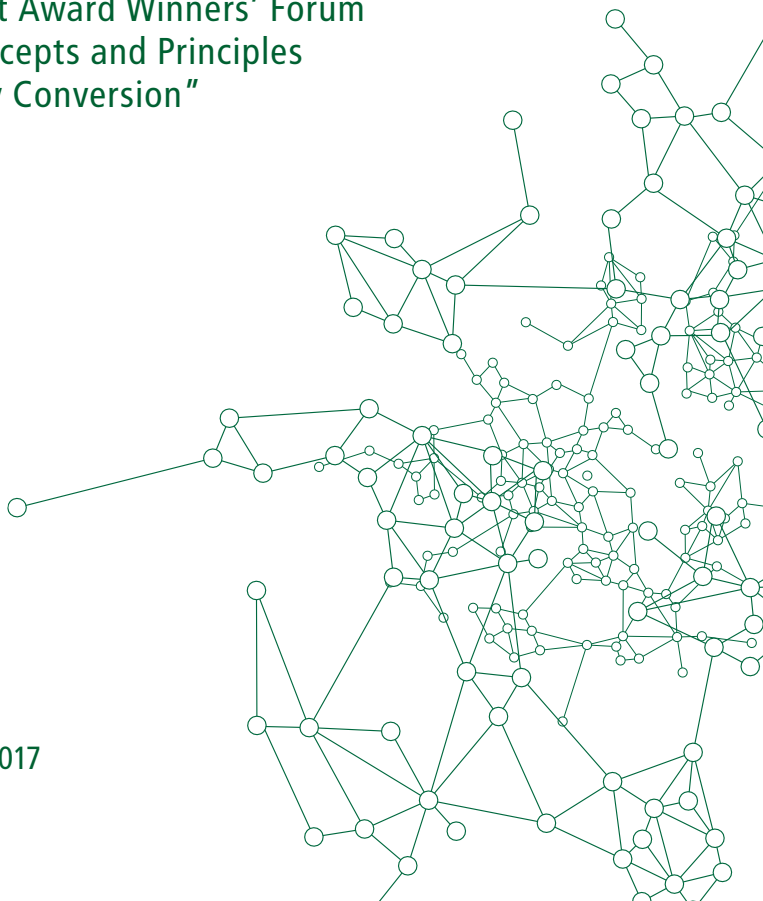
**Alexander von Humboldt**  
Stiftung/Foundation

# Programme

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7th Bonn Humboldt Award Winners' Forum  
"Fundamental Concepts and Principles  
of Chemical Energy Conversion"

Bonn, 11–15 October 2017



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**Bonn**

## 7th Bonn Humboldt Award Winners' Forum "Fundamental Concepts and Principles of Chemical Energy Conversion"

The conversion of energy for human activities will in the coming decades – independently from short-term political impulses – gradually change from fossil to renewable primary energy sources. In the case of the latter, the volatility and the need to serve various applications with molecular energy carriers requires the conversion of electricity into molecular "solar fuels", such as hydrogen from water or methanol from water or carbon dioxide, to name just two examples. We are far from understanding how to achieve this conversion with the same efficiency as the conversion of fuels into energy. The scale of these energy conversion methods approaches that of all other industrial material conversion processes together and represents the largest application of interfacial technologies, such as photo-, electro-, and chemo-catalysis.

The fundamental science behind this is a combination of nano- and interface science cutting through all chemistry disciplines, including i.e. the development of novel materials but also surface science, and links physics with chemistry. Biology contributes fundamental insights in the mechanisms of carbon cycles and further provides us with the function of collecting CO<sub>2</sub> without having to add extra energy besides sunshine.

Sustainable energy supply with renewable sources can only function if we open our mind to the systemic aspects of energy. The present division into compartments of energy usage groups, such as electricity, mobility, house heating with special regulatory frameworks each, is detrimental and precludes standardized societal and regulatory measures. These measures are at least as important for successful energy transformation as scientific concepts and principles. It will be the insight of present and future decision-makers on the fundamental and systemic aspects of energy supply that will determine success or failure of this transformation and thus, the future of mankind.

### Scientific Lead:

Professor Dr. Robert Schlögl  
Fritz Haber Institute of the Max Planck Society in Berlin

Professor Dr. Nicola Hüsing  
University of Salzburg

## Programme

### Wednesday, 11 October 2017

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from 3:00 p.m.	<b>Arrival and registration of the participants</b>	Hotel Bristol Prinz-Albert-Straße 2 53113 Bonn
		Hotel Residence Kaiserplatz 11 53113 Bonn
4:30 p.m.	<b>Walk from the hotels to the university</b>	Meeting Points: Hotel lobbies
5:00 p.m.	<b>Opening Ceremony</b>	Lecture Hall IX University of Bonn Regina-Pacis-Weg 3 53113 Bonn
	<b>Welcome and Opening Remarks</b>	
	Michael Hoch Rector of the University of Bonn	
	Angelica Maria Kappel Mayor of the City of Bonn	
	Helmut Schwarz President of the Alexander von Humboldt Foundation	
	<b>Keynote Lecture:</b> <b>"Design of Sustainable Catalytic Processes on Nanoporous Materials"</b>	
	Cynthia M. Friend Harvard University, Cambridge, USA	
afterwards	<b>Reception</b>	Säulenhalle University of Bonn
from 9:30 p.m.	<b>Walk from the university to the hotels</b>	

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## Thursday, 12 October 2017

from 8:00 a.m.	Registration	Hotel Bristol Bonn
9:00 a.m.	<b>Welcome and Introduction</b> Enno Aufderheide, Secretary General, Alexander von Humboldt Foundation	Conference Room "Chur I/II" Hotel Bristol Bonn
	<b>Welcome Address</b> Robert Schlögl, Fritz Haber Institute of the Max Planck Society Berlin, Germany	
	<b>Lectures – Panel I</b> Chair: Robert Schlögl, Fritz Haber Institute of the Max Planck Society Berlin	Conference Room "Chur I/II" Hotel Bristol Bonn
9:15 a.m.	<b>"Transition metal catalysts for energy technologies: Pathways to improve catalyst design"</b> Charles T. Campbell, University of Washington, Seattle, USA	
10:10 a.m.	<b>"Mass Transfer on Nanoscales: Insights, Surprises and Challenges"</b> Jörg Kärger, Universität Leipzig, Germany	
11:05 a.m.	Coffee and tea break	
11:35 a.m.	<b>"Status and recent findings in superconducting materials"</b> Robert J. Cava, Princeton University, USA	Conference Room "Chur I/II" Hotel Bristol Bonn
12:30 p.m.	Lunch	Restaurant Majestic

1:30 p.m.	<b>Lectures – Panel II</b>  <b>"Supercapacitors and electroactuators with ionic liquids: the essential physics at the nanoscale"</b> Alexei Kornyshev, Imperial College of Science, Technology and Medicine, Great Britain	Conference Room "Chur I/II" Hotel Bristol Bonn
2:25 p.m.	<b>Flashtalks/Poster Session of Humboldt Fellows and early career researchers with discussions</b> With coffee/tea and networking break	Conference Room "Chur I/II" Hotel Bristol Bonn
3:45 p.m.	<b>"Halide Perovskites: Poor man's new high performance semiconductors"</b> Mercouri G. Kanatzidis, Northwestern University, USA	Conference Room "Chur I/II" Hotel Bristol Bonn
4:40 p.m.	<b>"What can surface science tell us about the light harvesting properties of TiO<sub>2</sub>?"</b> Geoffrey Thornton, University College London, Great Britain	
5:35 p.m.	Break	
6:00 p.m.	Dinner	Restaurant Majestic
7:10 p.m.	Walk to Beethoven-Haus, Bonngasse 18-26, 53111 Bonn	Meeting Point: Hotel lobby Hotel Bristol Bonn
7:30 p.m.	<b>Lecture Recital</b> Professor Dr. William A. Kinderman, Piano University of Illinois at Urbana-Champaign, USA	Kammermusiksaal Beethoven-Haus Bonngasse 24-26 53111 Bonn
9:30 p.m.	Walk from Beethoven-Haus to the hotels	

## Friday, 13 October 2017

from 8:00 a.m.	Registration	Hotel Bristol Bonn
	<b>Lectures – Panel III</b> Chair: Nicola Hüsing, University of Salzburg, Austria	Conference Room "Chur I/II" Hotel Bristol Bonn
9:00 a.m.	<b>"Oxide reducibility in catalysis: From biomass conversion to CO oxidation"</b> Gianfranco Pacchioni, Università degli Studi di Milano-Bicocca, Italy	
9:55 a.m.	<b>"Energy Conversion at the Atomic Scale: 'Watching' Chemical Reactions, Molecule-by-Molecule"</b> Ulrike Diebold, Technical University Vienna, Austria	
10:50 a.m.	Coffee and tea break	
11:20 a.m.	<b>"Microscopic insights on fabrication and properties of functional components for energy devices using synchrotron-based methods"</b> Maya Kiskinova, Sincrotrone Trieste, Italy	Conference Room "Chur I/II" Hotel Bristol Bonn
12:15 p.m.	Lunch	Restaurant Majestic
1:30 p.m.	<b>"Photocatalysis for Water Splitting to H<sub>2</sub>: Mechanistic Insights"</b> Francisco Zaera, University of California, Riverside, USA	Conference Room "Chur I/II" Hotel Bristol Bonn
2:30 p.m.	<b>Flash Talks/Poster Session of Humboldt Fellows and Early Career Researchers with discussions</b> with coffee/tea and networking break	Conference Room "Chur I/II" Hotel Bristol Bonn

	<b>Lectures – Panel IV</b>	Conference Room "Chur I/II" Hotel Bristol Bonn
4:00 p.m.	<b>"Concepts and phenomena in heterogeneous photocatalysis. A surface chemist's view"</b> Elio Giamello, Università degli Studi di Torino, Italy	
4:55 p.m.	<b>"ABCO<sub>2</sub>"</b> Geoffrey A. Ozin, University of Toronto, Canada	
6:00 p.m.	Break	
7:00 p.m.	<b>Reception before Conference Dinner</b>	Lounge Hotel Bristol Bonn
7:30 p.m.	<b>Conference Dinner</b> <b>Dinner Speech "Chemical Energy Conversion: Thoughts of an industrial chemist"</b> Hartmann F. Leube, Senior Vice President "Process, Research and Chemical Engineering" BASF SE, Ludwigshafen, Germany	Restaurant Majestic

## Saturday, 14 October 2017

9:00 a.m.	Meeting at Hotel Bristol Joint Walk to Arithmeum	Hotel Bristol Prinz-Albert-Straße 2 53113 Bonn
9:30 a.m.	<b>Arithmeum – Tour through the collections</b> Welcome: Bernhard Korte, Director, Research Institute for Discrete Mathematics, University of Bonn, Germany Please note that a family tour in English will be available	Lennéstraße 2 53113 Bonn
11:00 a.m.	Joint walk to Alter Zoll landing pier	
11:30 a.m.	<b>Rhine River Cruise on the "Filia Rheni"</b> From Bonn to Remagen, including lunch break	
1:30 p.m.	Bus Transfer from Remagen to Bad Neuenahr	
2:15 p.m.	<b>Dokumentationsstätte Regierungsbunker – The Government Bunker</b> Please note that family tours in English will be available	
4:15 p.m.	Bus transfer to Weingut Meyer-Näkel (optional bus transfer directly back to Bonn available, arrival at Hotel Bristol appr. 5:15 p.m.)	
4:45 p.m.	<b>Wine tasting and farewell dinner</b> Weingut Meyer-Näkel, Dernau	Kloster Marienthal Klosterstraße 3-5 53507 Dernau
8:00 p.m.	Bus transfer to Bonn (arrival at Hotel Bristol appr. 9:30 p.m.)	Prinz-Albert-Straße 2 53113 Bonn

## Sunday, 15 October 2017

until 10:00 a.m. Checkout and Departure

## Poster Flash Talks

Session 1: 12 October 2017, 2:25 p.m.

- FT01 Dr. habil. Juras Banyas, Vilnius University  
"Dielectric Response of the Methylammonium Lead Halide Solar Cell Absorbers"
- FT02 Prof. Dr. Arnab Bhattacharya, Tata Institute of Fundamental Research  
"Novel semiconductor hybrid structures for energy conversion"
- FT03 Prof. Dr. Carlos F.O. Graeff, Universidade Estadual Paulista Julio de Mesquita Filho  
"Chemical Precursors for the deposition of thin solid films for solar energy harvesting and conversion: Advantages and limitations"
- FT04 Dr. Olga Kasian, Ukrainian State University of Chemical Technology  
"Mechanistic insights into water splitting on iridium-based anodes: in-situ observation of oxygen evolution and catalyst degradation intermediate"
- FT05 Dr. Zhe-Chen Wang, University of Colorado at Boulder  
"Reactivity of Bio-Molecule Anions in Space"
- FT06 Dr. Ralf Tonner, Philipps-Universität Marburg  
"Learning from Molecular Chemistry – Computational Materials Design"
- FT07 Dr. Camilla Evangelisti, Zentrum für Sonnenenergie und Wasserstoff-Forschung  
"Anticorrosion additive studies for Zinc-air Battery"
- FT08 Dr. Erwan Bertin, Universität Duisburg-Essen  
"Ligand-free Nanoparticles as Catalysts for Alkaline Fuel Cells"
- FT09 Dr. Albert Bruix Fuste, Technische Universität München  
"Multi-scale modeling of phase transitions and kinetic oscillations under steady-state and transient conditions"
- FT10 Dr. Shuangqiang Chen, Max-Planck-Institut für Festkörperforschung  
"Dual-functionalized double carbon shells coated silicon nanoparticles for high performance lithium ion batteries"
- FT11 Montaha Anjass, Ulm University  
"New molecular vanadium oxides as high-performance lithium ion battery electrodes"
- FT12 Severin Vierrath, University of Freiburg  
"Novel approaches to tailor the PEM | electrode interface for increased power density"

## Poster Flash Talks

Session 2: 13 October 2017, 2:30 p.m.

- FT13 Prof. Matteo Maestri, Politecnico di Milano  
"Morphological changes of catalyst materials in reacting conditions by combined ab-initio thermodynamics and microkinetic modeling"
- FT14 Dr. Subhendu Kumar Panda, CSIR Central Electrochemical Research Institute  
"Metal sulfide nanostructures as efficient counter electrodes for dye-sensitized solar cells"
- FT15 Prof. Dr. K. Christian Teichert, Montanuniversität Leoben  
"Organic semiconductor nanstructure devices on two-dimensional materials"
- FT16 Prof. Dr. Zhenyu Tian, Chinese Academy of Sciences  
"Chemical Kinetics of Homo- and Heterogeneous Combustion"
- FT17 Prof. Dr.-Ing. Rafiqul Islam, University of Dhaka  
"Chemical Energy Conversion of Coal in the Underground Coal Gasification Process to mitigate climate change as well as energy and fertilizer shortages in Bangladesh"
- FT18 Dr. Artur P.N. Erbe, Helmholtz-Zentrum Dresden-Rossendorf e.V.  
"Electronic nanostructures by combining top-down and bottom-up strategies"
- FT19 Dr. Lars Heinke, Karlsruher Institut für Technologie  
"Photoswitchable Nanoporous Films for Continuously Tunable Membrane Separation"
- FT20 Dr. Ursula Wurstbauer, Technische Universität München  
"Photocatalytic properties of individual MoS<sub>2</sub> crystals for HER"
- FT21 Dr. Thomas Kadyk, TU Braunschweig  
"Flight Path Fuel Cell: Future Aviation Based On Electrochemistry"
- FT22 Dr. Ye Yu, Leibniz-Institut für Polymerforschung Dresden e.V.  
"Manipulating Photon Upconversion with Optical Cavity"
- FT23 Josefine Hildebrand, Carl von Ossietzky Universität  
"Sol gel synthesis of doped titanates with specific modified stoichiometry for CO<sub>2</sub> reduction"
- FT24 Dr. Martin Schmid, Philipps-Universität Marburg  
"Interphase Formation in Organic Semiconductor Films Examined with Hard X-ray Photoelectron Spectroscopy"

## Poster Sessions

12 and 13 October 2017

- P01 Montaha Anjass, Ulm University  
"New molecular vanadium oxides as high-performance lithium ion battery electrodes"
- P02 Dr. habil. Juras Banys, Vilnius University  
"Dielectric Response of the Methylammonium Lead Halide Solar Cell Absorbers"
- P03 Markus Becker, Carl von Ossietzky University Oldenburg  
"Morphology Control of Planar Heterojunction Perovskite Solar Cells and Ab-Initio Steric Engineering of the ABX<sub>3</sub> Crystal Structure"
- P04 Dr. Yonder Antonio Berencen Ramirez, Helmholtz-Zentrum Dresden-Rossendorf  
"Controlled ion beam hyperdoping of silicon nanowires"
- P05 Dr. Erwan Bertin, Universität Duisburg-Essen  
"Ligand-free Nanoparticles as Catalysts for Alkaline Fuel Cells"
- P06 Prof. Dr. Arnab Bhattacharya, Tata Institute of Fundamental Research  
"Novel semiconductor hybrid structures for energy conversion"
- P07 Dr. Albert Bruix Fuste, Technische Universität München  
"Multi-scale modeling of phase transitions and kinetic oscillations under steady-state and transient conditions"
- P08 Dr. Viktor Brus, Helmholtz-Zentrum Berlin für Materialien und Energie  
"Temperature switchable type of conductivity in conjugated polyelectrolyte/graphene two-dimensional nanocomposites"
- P09 Dr. Shuangqiang Chen, Max-Planck-Institut für Festkörperforschung  
"Dual-functionalized double carbon shells coated silicon nanoparticles for high performance lithium ion batteries"
- P10 Dr. Artur P. N. Erbe, Helmholtz-Zentrum Dresden-Rossendorf e.V.  
"Electronic nanostructures by combining top-down and bottom-up strategies"
- P11 Dr. Camilla Evangelisti, Zentrum für Sonnenenergie und Wasserstoff-Forschung  
"Anticorrosion additive studies for Zinc-air Battery"
- P12 Dr. Hongyu Gao, Universität des Saarlandes  
"A new force field developed for interfacial interactions between graphene and hexadecane"

- P13 Prof. Dr. Carlos F.O. Graeff, Universidade Estadual Paulista Julio de Mesquita Filho  
"Chemical Precursors for the deposition of thin solid films for solar energy harvesting and conversion: Advantages and Limitations"
- P14 Dr. Ritesh Haldar, Karlsruher Institut für Technologie  
"Excitonic coupling and transport in Metal-organic thin films"
- P15 Dr. Lars Heinke, Karlsruher Institut für Technologie  
"Photoswitchable Nanoporous Films for Continuously Tunable Membrane Separation"
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- P19 Dr. Olga Kasian, Ukrainian State University of Chemical Technology  
"Mechanistic insights into water splitting on iridium-based anodes: in-situ observation of oxygen evolution and catalyst degradation intermediate"
- P20 Dr. Yanyu Liang, Nanjing University of Aeronautics and Astronautics  
"MOFs-derived Oxygen Reduction Electrocatalysts: From Nanostructure Control to Catalytic Mechanism Insights"
- P21 Dr. Anna Lyamkina, Technische Universität München  
"Plasmon-exciton interaction in systems with monolithically integrated InAs/AlGaAs quantum dots"
- P22 Prof. Matteo Maestri, Politecnico di Milano  
"Morphological changes of catalyst materials in reacting conditions by combined ab-initio thermodynamics and microkinetic modeling"
- P23 Dr. Charlene Ng, Leibniz-Institut für Polymerforschung Dresden e.V.  
"Partially Embedded Plasmonic Nanoparticles within Semiconductors for Enhanced Hot Carrier Extraction"

- P24 Dr. Subhendu Kumar Panda, Central Electrochemical Research Institute  
"Metal sulfide nanostructures as efficient counter electrodes for dye-sensitized solar cells"
- P25 Dr. Antonio Otavio Patrocinio, Gottfried Wilhelm Leibniz Universität Hannover  
"Layer-by-layer thin films of hexaniobate nanoscrolls as effective photocatalysts for H<sub>2</sub> evolution"
- P26 Dr. Martin Schmid, Philipps-Universität Marburg  
"Interphase Formation in Organic Semiconductor Films Examined with Hard X-ray Photoelectron Spectroscopy"
- P27 Prof. Dr. K. Christian Teichert, Montanuniversität Leoben  
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"Photocatalytic properties of individual MoS<sub>2</sub> crystals for HER"
- P33 Dr. Ye Yu, Leibniz-Institut für Polymerforschung Dresden e.V.  
"Manipulating Photon Upconversion with Optical Cavity"



# General Information

## Conference Venues and Hotels

Günnewig Hotel Bristol Bonn  
Prinz-Albert-Str. 2  
53113 Bonn

Tel.: +49 (0)228 26 98-0

Fax: +49 (0)228 26 98-2 22

E-Mail: [bristol.bonn@guennewig.de](mailto:bristol.bonn@guennewig.de)

[www.guennewig.de/bnbristo](http://www.guennewig.de/bnbristo)

Günnewig Hotel Residence  
Kaiserplatz 11  
53113 Bonn

Tel.: +49 (0)228 26 97-0

Fax: +49 (0)228 26 97-7 77

E-Mail: [hotel.residence@guennewig.de](mailto:hotel.residence@guennewig.de)

[www.guennewig.de/bnreside](http://www.guennewig.de/bnreside)

University of Bonn  
Regina-Pacis-Weg 3  
53113 Bonn

## Hotel Reservation

Please check out of your room on departure day no later than 11:00 a.m. If you wish to arrange for a late departure, please contact the Welcome Desk. Please note that all extra charges (e.g. for telephone, parking, taxi, and room service) are at your own expense.

## Meals

Breakfast will be served between 6:30 a.m. and 10:30 a.m. Organised meals start with the reception on 11 October 2017 and end with the farewell dinner at the winery on 14 October 2017.

## WiFi Access during the Symposium

The hotels Bristol and Residence provide free WiFi access in the entire hotel.

## Smoking

Please note that smoking is not permitted in the hotels.

## Disclaimer

Please note that participation takes place at your own risk. We ask for your understanding that neither the Alexander von Humboldt Foundation nor lab concepts GmbH are liable for any losses, accidents or damages, irrespective of which cause, to people and property during travel as well as during the conference.

## Photographer during the Conference

We would like to inform you that a photographer contracted by the Alexander von Humboldt Foundation will be present at the Humboldt Award Winners' Forum. The photographs taken may be published by the Alexander von Humboldt Foundation for the purpose of information and public relations work as well as being published on the Foundation's internal social network. They will not be used for commercial purposes. If you do not agree with the publication of photographs in which you feature, please inform us no later than 6 October 2017 by sending an email to Nina Hafeneger ([nina.hafeneger@avh.de](mailto:nina.hafeneger@avh.de)).

## Name Tags

Upon registration, you will receive a name tag. Please wear it during the entire conference, it will make it easier for all participants to address each other.

## How to Recognise the Participants

	<b>Yellow</b>	Research Award Winners
	<b>Green</b>	Research Fellows
	<b>Blue</b>	Alumni
	<b>Light Blue</b>	Junior Researchers
	<b>Beige</b>	Academic Hosts
	<b>Grey</b>	Members of the Selection Committees
	<b>Orange</b>	Spouses and Partners
	<b>White</b>	Guests
	<b>Bordeaux</b>	Staff of the Alexander von Humboldt Foundation

### **Organiser**

Alexander von Humboldt Foundation  
Jean-Paul-Straße 12  
53173 Bonn, Germany  
Tel./Phone: +49 (0)228 / 833-0  
Fax: +49 (0)228 / 833-199  
Email: [info@avh.de](mailto:info@avh.de)  
[www.humboldt-foundation.de](http://www.humboldt-foundation.de)

### **Organisation**

labconcepts GmbH  
Bonner Talweg 64  
53113 Bonn  
Tel./Phone: +49 (0)228 / 24 98 110  
Fax: +49 (0)228 / 24 98 111  
E-Mail: [humboldt-forum@lab-concepts.de](mailto:humboldt-forum@lab-concepts.de)  
[www.labconcepts.de](http://www.labconcepts.de)

### **Contact during the Conference**

Sandra Mayer  
Phone: +49 (0)163 96 77 739



**Alexander von Humboldt**  
Stiftung/Foundation

Jean-Paul-Str. 12  
D-53173 Bonn

Tel.: +49 (0) 228 833-0  
Fax: +49 (0) 228 833-199

E-Mail: [info@avh.de](mailto:info@avh.de)

[www.humboldt-foundation.de](http://www.humboldt-foundation.de)