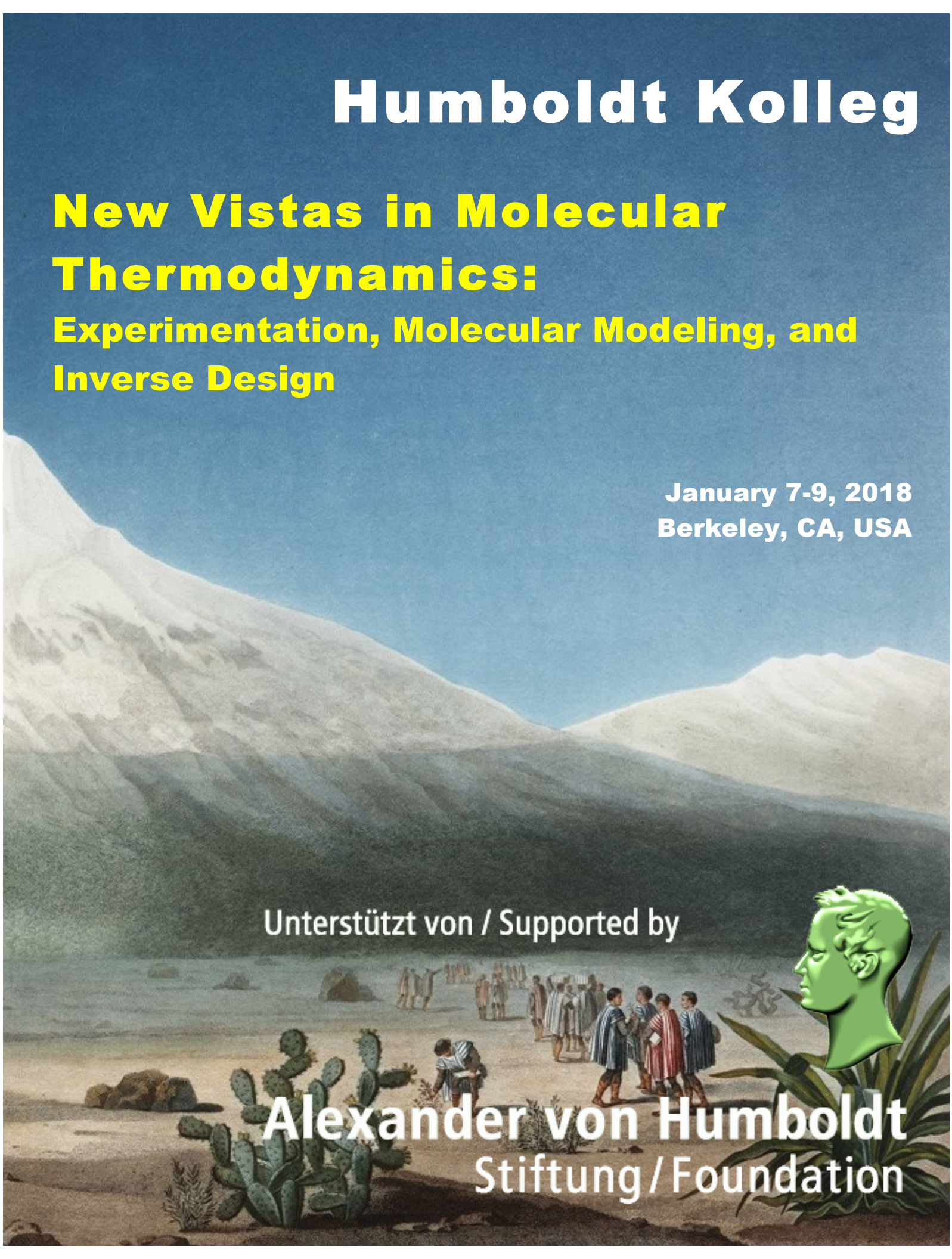
Humboldt Kolleg

New Vistas in Molecular Thermodynamics:

Experimentation, Molecular Modeling, and Inverse Design

January 7-9, 2018
Berkeley, CA, USA



Prologue

The past few decades have witnessed the advent of molecular engineering, cyberspace and artificial intelligence. These new technological developments obscure the boundaries among traditional disciplines of science and engineering. By advocating interdisciplinary and international communication, the Humboldt Kolleg aims to identify common interests in fundamentals, enhance mutual understanding and promote collaborations among researchers from sub-areas of the molecular-thermodynamics community.

Molecular thermodynamics has been an enabling tool to accelerate scientific innovations, to catalyze emerging technologies, and to provide core knowledge for design and optimization of diverse industrial systems ranging from energy production, materials synthesis, and chemical processing to pharmaceutical and environmental applications. Whereas the number of investigators in molecular thermodynamics, especially in computation and molecular modeling, has increased much in recent years, the field is diverging into numerous specialized branches that focus on specific systems of interest (e.g., fluids vs. solids), methodology (e.g., experiment vs. molecular theory and modeling), or applications (e.g., materials vs. biotechnology), and different scales of thermodynamic problems (e.g., nano vs. meso vs. macro). Sponsored by the Alexander von Humboldt Foundation, this workshop aims to advocate closer collaborations among experiment, modeling and computational research in molecular thermodynamics. By providing a forum for participants from different disciplines of science and engineering, ranging from experimentation, modeling and machine learning, we hope that this workshop may help define new frontiers in molecular thermodynamics, challenge the current thinking of engineering research beyond curiosity-driven exploration, and perhaps begin to build new roadmaps for data-based rational design of chemical processes, products, materials and devices.

Organizers:
Jianzhong Wu, University of California, Riverside
Joan Brennecke, University of Texas, Austin

Alexander von Humboldt
Stiftung/Foundation

Humboldt Kolleg

January 7-9, 2018, Berkeley, USA

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Sunday, January 7, 2018

5:00 pm – 5:30 pm	**Registration**	Tan Hall Lobby
5:30 pm – 8:30 pm	**Poster and Networking**	Tan Hall Lobby
	Nora Spanish Catering, Beverages from Germany and California	

Monday, January 8, 2018

8:30 am – 9:00 am **Welcome and Opening Remarks** 180 Tan Hall

Douglas Clark
College of Chemistry Dean, University of California, Berkeley

Ulrike Albrecht
Head of Department Strategy and External Relations
Alexander von Humboldt Foundation

Jianzhong Wu
Department of Chemical Engineering, University of California, Riverside

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9:00 am – 11:30 am **Fundamentals of Chemical Design and Engineering** 180 Tan Hall

Moderator: Zhen-Gang Wang
Department of Chemical Engineering, Caltech

Alán Aspuru-Guzik
Department of Chemistry and Chemical Biology, Harvard University

Rigoberto Hernandez
Department of Chemistry, Johns Hopkins University

Giulio C. Sarti
DICAM -Università di Bologna, Italy

Kai Leonhard
Lehrstuhl für Technische Thermodynamik, RWTH Aachen University

Panel Discussion

11:30 am – 1:00 pm **Lunch Break** Faculty Club

1:00 pm – 3:30 pm **Exploring the Chemical Space** 180 Tan Hall

Moderator: Daniel Lambrecht
Department of Chemistry, University of Pittsburgh

Brenda Rubenstein
Department of Chemistry, Chemistry, Brown University

Alpha Lee
Department of Chemistry, Cambridge University, UK

Volker Blum
Department of Mechanical Engineering and Materials Science, Duke University

Hans Kistenmacher
Innovation Management, Linde Group, Germany

Panel Discussion

3:30 pm – 4:00 pm **Coffee/Tea and Networking Break** Tan Hall Lobby

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4:00 pm – 6:30 pm **Energy Conversion & Storage** 180 Tan Hall

Moderator: Peter Cummings
Department of Chemical Engineering, Vanderbilt University

Martin Z. Bazant
Department of Chemical Engineering/Mathematics, MIT

Randall Q. Snurr
Department of Chemical and Biological Engineering, Northwestern University

Xiaoyan Ji
Division of Energy Science, Luleå University of Technology

Rui Qiao
Department of Mechanical Engineering, Virginia Tech

Panel Discussion

7:00 pm – 9:30 pm **Conference Dinner** Seaborg Room/ Faculty Club

Dinner speaker: Jeffrey A. Reimer
Chair, Department of Chemical and Biomolecular Engineering
University of California, Berkeley

Tuesday, January 9, 2018

8:30 am – 11:30 am **Materials by Design** 180 Tan Hall

Moderator: Michael Deem
Department of Bioengineering, Rice University

Juan de Pablo
Institute for Molecular Engineering, University of Chicago

Nitash P. Balsara
Department of Chemical & Biomolecular Engineering, University of California Berkeley

David Sholl
Department of Chemical Engineering, Georgia Institute of Technology

Marcus Müller
Institute of Theoretical Physics, the University of Göttingen

Jianwen Jiang
Department of Chemical & Biomolecular Engineering, National University of Singapore

Panel Discussion

11:30 am – 1:00 pm **Lunch Break** Faculty Club

1:00 pm – 3:30 pm **Biotechnology & Pharmaceutics** 180 Tan Hall

Moderator: John O'Connell
Department of Chemical Engineering, University Virginia

Gabriele Sadowski
Department of Chemical Engineering, Technische Universität, Dortmund

Andy Spakowitz
Department of Chemical Engineering, Stanford University

Stefan M. Kast
Theoretische Physikalische Chemie, Technische Universität Dortmund

Carol K. Hall
Department of Chemical and Biomolecular Engineering, North Carolina State University

Panel Discussion

3:30 pm – 4:00 pm **Coffee/Tea and Networking Break** Tan Hall Lobby

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4:00 pm – 6:30 pm **Engineering Molecular Thermodynamics** 180 Tan Hall

Moderator: Christoph Held
Department of Chemical Engineering, Technische Universität, Dortmund

Joan Brennecke
Department of Chemical Engineering, University of Texas at Austin

Walter Chapman
Department of Chemical Engineering, Rice University

Xiaohua Lu
School of Chemical Engineering, Nanjing Tech University, China

Keith E. Gubbins
Department of Chemical and Biomolecular Engineering, North Carolina State University

Panel Discussion

6:30 pm – 7:00 pm **Closing Remarks** 180 Tan Hall

John M. Prausnitz
Department of Chemical and Biomolecular Engineering
University of California, Berkeley

Notes

General Information

Conference Venue
1st Floor, Tan Kah Kee Hall
University of California at Berkeley
Berkeley, CA 94720-1462

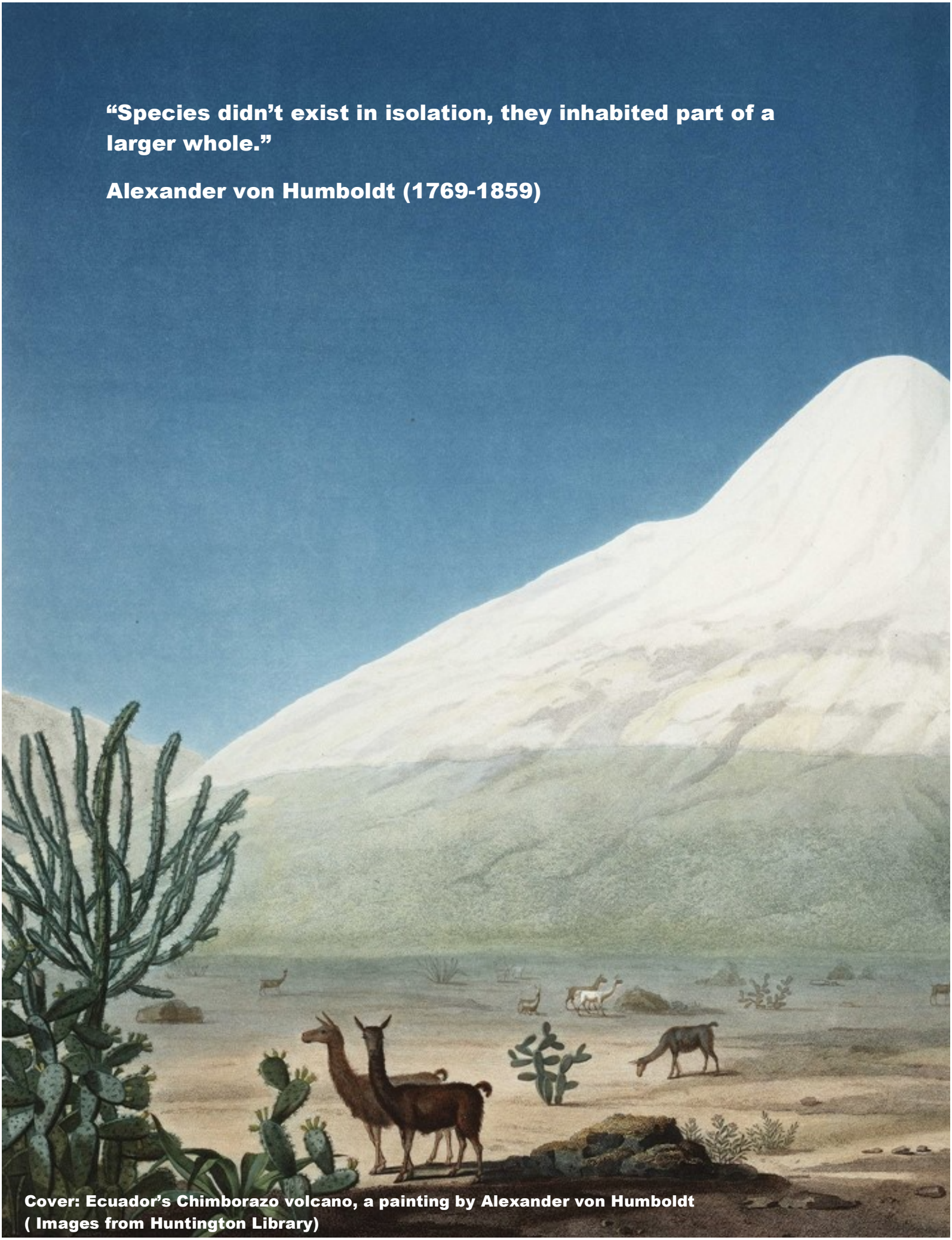
Registration and Nametags
Each participant will be given a nametag upon registration. Please wear it during the entire meeting so that it will be easier for all participants to address each other.

The forms for partial reimbursement/honorarium will be available at the registration desk.

Meals
Lunch tickets are available at registration on Sunday night, January 7th, 2018.

“Species didn’t exist in isolation, they inhabited part of a larger whole.”

Alexander von Humboldt (1769-1859)



Cover: Ecuador’s Chimborazo volcano, a painting by Alexander von Humboldt (Images from Huntington Library)