Telluride Science Research Center – Summer 2015

Workshop
"Clathrate Hydrates Fundamentals: Bridging Molecular Structures to Microscopic Properties and Behavior"

Dates
07/06/2015 - 07/10/2015

Organizers
Amadeu Sum, Colorado School of Mines
John Tse, University of Saskatchewan
Zlatko Bacic, New York University

TSRC Host
Mark Kozak

Meeting Description
Clathrate hydrates are crystalline inclusion compounds formed from the hydrogen bonding of water molecules (host) enclosing relative small molecules (guest). These structures have unique properties that originate from molecular interactions of the host and guest molecules. Much fundamental knowledge has been gained on clathrate hydrates, especially from the combination of microscopic tools aimed at probing the molecular interactions, both equilibrium and transient, using spectroscopy, diffraction, ab initio calculations, molecular simulations, and theory. This workshop aims to gather a mix of experimental, theoretical, and simulation researchers to state and discuss the latest findings and challenges on clathrate hydrates at the microscopic level. Particular emphasis are given in the synergism to be gained by stimulating discussion among experimentalists, theoreticians, and simulators in the topics of interest include, but not limited to, nucleation and growth, guest-host interactions, guest and host dynamics, structure-properties relations, unusual guests/structure.

Location
Telluride Elementary School
477 West Columbia Ave, Telluride, CO 81435

Workshop Schedule

Monday, July 6

8:00 am - 8:30 am	Breakfast at TSRC
8:30 am - 11:30 am	Presentations/ Discussion I
11:30 am - 3:00 pm	Lunch / Free time
3:00 pm - 6:00 pm	Presentations/Discussions II
7:00 pm	Group dinner at local restaurant (family welcome) - optional

Tuesday, July 7

8:00 am - 8:30 am	Breakfast at TSRC
8:30 am - 11:30 am	Presentations/Discussions IIII
11:30 am - 2:00 pm	Lunch / Free time
2:00 pm - 5:00 pm	Presentations/Discussions IV
6:00 pm - 7:15 pm	TSRC Town Talk at the Conference Center in Mountain Village
8:00 pm	Group dinner at local restaurant (family welcome) - optional

Wednesday, July 8

8:00 am - 12:00 pm	Morning free for hiking/free-time
2:00 pm - 5:00 pm	Presentations/Discussions V
6:00 pm - 9:00 pm	TSRC Picnic @ Telluride Elementary School, under the tent

Thursday, July 9

8:00 am - 8:30 am	Breakfast at TSRC
8:30 am - 11:30 am	Presentations/Discussions VI
11:30 am - 3:00 pm	Lunch / Free time
3:00 pm - 6:00 pm	Presentations/Discussions VII
7:00 pm	Group dinner at local restaurant (family welcome) - optional

Presentations/Discussions I – Session chair: TBD

Paul Brumby	"Equilibrium cage occupancies of SI methane hydrate by Gibbs ensemble Monte Carlo simulation"
Satoshi Takeya	"Distribution of guest molecules within clathrate hydrate cages determined by powder X-ray diffraction method"
Fulong Ning	"Mechanical Instability of Polycrystalline Methane Hydrates: Enlightenment from MD Simulation"

Presentations/Discussions II – Session chair: TBD

Peter Felker	"Translation-Rotation Dynamics of Clathrate-Entrapped Dihydrogen Clusters"
Lorenzo Ulivi	"Experiments on Hydrogen Clathrates: Formation, Stoichiometry and Quantum Dynamics"
Zlatko Bacic	"Molecular hydrogen in clathrate hydrates: quantum dynamics, condensed-phase effects, and inelastic neutron scattering spectra"

Presentations/Discussions III – Session chair: TBD

Barbara Wyslouzil	"Following ice and clathrate formation on the microsecond timescale"
Niall English	"MD simulation of clathrate-hydrate crystallisation and hydrate equilibrium time-dependent properties"
Amadeu Sum	"Nucleation of Clathrate Hydrates: How Far Have Has the Field Advanced?"

Presentations/Discussions IV – Session chair: TBD

Sotiris Xantheas	"Structure, gas accommodation and dynamical processes in clathrate hydrates lattices"
J. Paul Devlin	"HX molecules in clathrate-hydrate small cages: Controlling defect populations and formation rates with strong acids"
Motoi Yamada	"Vibrational analysis of guest molecule in clathrate hydrate with density functional theory"

Presentations/Discussions V – Session chair: TBD

Arnaud Desmedt	"Tuning the acidity of THF clathrate hydrates for improving hydrogen storage properties"
Toshiaki Iitaka	"Vibrational properties of rare gas hydrate"

Tianshu Li "Modeling gas hydrate nucleation by forward flux sampling method"

Presentations/Discussions VI – Session chair: TBD

Hsuan Lo "Can Molecular Dynamics Simulation Provide Quantitative Description for The Rate of Methane Hydrate Dissociation?"

Kenneth Janda "Formation kinetics of propane and difluoromethane clathrate hydrate"

Daisuke Yuhara "Analysis of nucleation and phase equilibrium of methane hydrate by molecular dynamics simulation"

Presentations/Discussions VII – Session chair: TBD

Shiang-Tai Lin "Nucleation and Growth of Methane+Tetrahydrofuran Mixed Guest Hydrates from Molecular Dynamic Simulations"

Kyle Hall "Nucleation of Binary Hydrates: A Molecular Dynamics Study"

Zhengcai Zhang "Multiple Pathways for Methane Hydrate Nucleation"

Note: The purpose of the presentation is to stimulate discussion. Each contribution will have 60 minutes. The presentation should be no longer than 45 minutes, leaving the remaining time for questions/discussion.

List of Participants

Amadeu Sum	Colorado School of Mines
Arnaud Desmedt	CNRS-ISM
Barbara Wyslouzil	Ohio State University
Daisuke Yuhara	Keio University
Fulong Ning	China University of Geosciences
Hsuan Lo	National Taiwan University
J. Paul Devlin	Oklahoma State University
Kenji Yasuoka	Keio University
Kenneth Janda	University of California, Irvine
Kyle Hall	University of Calgary
Lorenzo Ulivi	CNR-ISC
Motoi Yamada	Keio University
Niall English	University College Dublin
Paul Brumby	Keio University
Peter Felker	UCLA
Satoshi Takeya	National Institute of Advanced Industrial Science
Shiang-Tai Lin	National Taiwan University
Sotiris Xantheas	Pacific Northwest National Laboratory
Tianshu Li	George Washington University
Toshiaki Iitaka	RIKEN
Zhengcai Zhang	Chinese Academy of Sciences, Institute of Geology
Zlatko Bacic	New York University