

## CLATHRATE HYDRATES FUNDAMENTALS: Bridging Molecular Structures to Microscopic Properties and Behavior

ORGANIZER NAMES: David WU and Arnaud DESMEDT

LOCATION: Telluride Intermediate School, 725 W Colorado Ave Telluride CO, 81435

	Tuesday	Wednesday	Thursday	Friday	Saturday
TIME	juin-20	juin-21	juin-22	juin-23	juin-24
8:30-9:00	Breakfast	Breakfast	Breakfast	Breakfast	Breakfast
9:00 - 9:45	Welcome (9:30)	Session 2 / R. Bauer	Session 4 / B. Peters	Session 5 / Z. Bacic	Session 6 / K. Yasuoka
9:45 - 10:30	Session 1 / W. Kuhs	Session 2 / S.S. Lee	Session 4 / T. Li	Session 5 / B. Chazallon	Session 6 / P. Brumby
	<i>Discussion + Break</i>	<i>Discussion + Break</i>	<i>Discussion + Break</i>	<i>Discussion + Break</i>	<i>Discussion + Break</i>
11:00 - 11:45	Session 1 / M. Matsumoto	Session 2 / N. English	Session 4 / S. Sarupria	Session 5 / L. Bove	Session 6 / B. Bouillot
11:45 - 12:30	group discussion	group discussion	group discussion	Session 5 / A. Desmedt	Concluding remarks
	<i>Lunch</i>	<i>Lunch</i>	<i>Lunch</i>	<i>Lunch</i>	<i>END at 12.00</i>
2:30 - 3:15	Session 1 / E. Engel	Session 3 / A. Sum		Session 6 / P. Kusalic	
3:15 - 4:00	Session 1 / T. Hasegawa	Session 3 / S. Takeya		Session 6 / D. Wu	
	<i>Discussion + Break</i>	<i>Discussion + Break</i>	<i>Free afternoon</i>	<i>Discussion + Break</i>	
4:30 - 5:15	Session 1 / F. Ning	Session 3 / C. Petuya		group discussion	
5:15 - 5:45	group discussion	group discussion			
	<i>Break</i>	<i>Break</i>		<i>Break</i>	
		<b>EVENING SESSION</b>	<b>EVENING SESSION</b>	<b>EVENING SESSION</b>	
6:00 - 7:00	<i>Free evening</i>	<b>TOWN TALK</b>	<b>TELLURIDE PICNIC</b>	<b>GROUP DINNER</b>	
7:00 ...					

## Program – Telluride, June 2017

### **CLATHRATE HYDRATES FUNDAMENTALS: Bridging Molecular Structures to Microscopic Properties and Behavior**

#### **Session 1 : Ice/hydrate nucleation and dissociation**

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- **W. Kuhs** - University of Goettingen, Germany.  
*The role of gas hydrate crystal sizes, grain boundary networks, crystalline surfaces and interfaces.*
- **M. Matsumoto** - Okayama university, Japan.  
*Hypothetical new kind of ices at negative and very high pressures.*
- **E. Engel** – University of Cambridge, UK.  
*Mapping uncharted territory in ice and clathrate hydrates.*
- **T. Hasegawa** - Keio University, Japan.  
*Molecular dynamics simulation for the dissociation process of carbon dioxide hydrates*
- **F. Ning** - Colorado School of Mines, US.  
*Molecular Insights into Mechanical Strength of Polycrystalline Water Ice Containing Methane Hydrate Grains.*

#### **Session 2 : Role of surfaces and heterogeneous nucleation**

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- **R. Bauer** - University of Saskatchewan, Canada.  
*Clathrate Hydrate Nucleation from an Amorphous Solid Mixture.*
- **S.S. Lee** - Argonne National Laboratory, US.  
*Hydration Structure of Solid–Water Interfaces.*
- **N. English** – University College Dublin, Ireland.  
*Hydrogen-hopping in gas hydrates and methane-hydrate nucleation in marine environments: insights from biased molecular-dynamics.*

#### **Session 3 : Bulk structure**

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- **A. Sum** – Colorado School of Mines, US.  
*What We Know and Do Not Know About Xenon Hydrates.*
- **S. Takeya** - AIST, Japan.  
*Distribution of guest molecules within clathrate hydrate cages determined by powder X-ray diffraction.*
- **C. Petuya** – University of Bordeaux, France.  
*Metastability, guest partitioning and selective gas trapping in the mixed CO/N<sub>2</sub> clathrate hydrates.*

#### **Session 4 : Advanced sampling in simulations**

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- **B. Peters** - University of California, Santa Barbara, US.  
*Accelerated Nucleation and Polymorph Selection with Trace Additives: Theory and Simulation.*
- **T. Li** - George Washington University, US.  
*New molecular insights into the nucleation of ice and clathrate hydrate.*
- **S. Sarupria** – Clemson University, US.  
*Elucidating the molecular ballet of gas hydrates using computer simulations.*

## Session 5 : Quantum and spectroscopic properties

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- **Z. Bacic** - New York University, US.  
*Quantum translation-rotation dynamics, spectroscopy, and diffusion of hydrogen molecules in the condensed-phase environment of clathrate hydrates.*
- **B. Chazallon** – University of Lille, France.  
*Raman spectroscopy of gas hydrates: from fundamental aspects to chemical engineering applications with CO<sub>2</sub> capture technology.*
- **L. Bove** – CNRS - Univ. P.&M. Curie, France.  
*Guest dynamics in methane and hydrogen hydrates under extreme conditions.*
- **A. Desmedt** – CNRS – University of Bordeaux, France.  
*Strong acid clathrate hydrates: from fundamentals to applications.*

## Session 6 : Nucleation of mixtures

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- **P. Kusalik** - University of Calgary, Canada.  
*Characterizing Key Features in the Mechanism of Hydrate Nucleation.*
- **D. Wu** – Colorado School of Mines, US.  
*Molecular simulation of the nucleation of ethane hydrate and ethane/methane hydrate.*

## Session 7 : Thermodynamics and stability

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- **K. Yasuoka** - Keio University, Japan.  
*Isometric-Isothermal Molecular Dynamics Simulation of Methane Hydrate/Water/Methane Coexistence Systems.*
- **P. Brumby** – Keio University, Japan.  
*Isothermal-isobaric Gibbs ensemble Monte Carlo simulations of various clathrate hydrates.*
- **B. Bouillot** – Saint-Etienne School of Mines, France.  
*Investigation of Non-equilibrium Crystallization of Mixed Clathrate Hydrates: Experimental and Modeling Approaches.*