

Tuesday, October 18th, Meeting Schedule

Morning Session: Argonne National Lab., Building 241

8:00 – 8:30am Executive Session: SAB & Management Team (Room B-123)

8:30 – 8:45am Welcome by Peter Littlewood, ANL

8:45 – 9:15am Overview of the Center
Giulia Galli, The University of Chicago & ANL

Chair:
Clotilde Lethiec

9:15 – 9:30am General Discussion

9:30 – 10:00am Software Task (I)
François Gygi, University of California - Davis

10:00 – 10:30am Software Task (II)
Juan de Pablo, The University of Chicago & ANL

10:30 – 11:00am COFFEE BREAK

11:00 – 11:30am Validation Task
John Mitchell, ANL

11:30 – 12:00pm Data Task
Nicola Ferrier, ANL

12:00 – 1:30pm LUNCH

1:30 – 2:00pm SAB Closed Session (Room B-123)

Tuesday, October 18th, Meeting Schedule

Afternoon Session: Argonne National Lab., Building 241

- Scientific highlights (10 min + 5 min discussion) -

2:00 – 2:15pm	Computational Spectroscopy: WEST Marco Govoni, The University of Chicago & ANL	Chair: John Mitchell
2:15 – 2:30pm	Spectroscopy of Hydrogen-Bonded Liquids Alex Gaiduk, The University of Chicago	
2:30 – 2:45pm	Coarse Grained Molecular Dynamics for Ions in Heterogeneous Media Monica Olvera de la Cruz, Northwestern University	
2:45 – 3:00pm	A Validated Understanding of Solid-Liquid Interfaces Paul Fenter, ANL	

3:00 – 3:30pm COFFEE BREAK

3:30 – 3:45pm	SSAGES: New Sampling Methods and Applications Jonathan Whitmer, University of Notre Dame	Chair: Juan de Pablo
3:45 – 4:00pm	COPSS – Continuum Particle Simulation Suite Xikai Jiang, ANL	
4:00 – 4:15pm	Age and Structure of a Model Vapor-Deposited Glass Daniel Reid, The University of Chicago	
4:15 – 4:30pm	Three Dimensional Metrology using Molecular Simulation and X-Ray Scattering Alec Bowen, The University of Chicago	
4:30 – 4:45pm	Nanoparticle Validation Dmitri Talapin, The University of Chicago	
4:45 – 5:00pm	Concluding Remarks Giulia Galli, The University of Chicago & ANL	
5:00 – 7:00pm	Poster Session - Wine and Cheese	

7:30pm Dinner – SAB and Management Team
Cooper's Hawk, Naperville, IL

Wednesday, October 19th, Meeting Schedule

Morning Session: Argonne National Lab., Building 241

9:00 – 10:00am	Advisory Board Breakfast and Discussion Preparation of Report (Closed Session – Room B-123)
10:00 – 11:00am	SAB & Management Team meeting
In parallel	
9:00 – 11:00am	Junior Retreat (Room D-172)
11:00 – 11:30am	Future directions Giulia Galli, The University of Chicago & ANL
11:30 – 11:45am	Concluding Remarks Matthew Tirrell, The University of Chicago & ANL
12:00 – 1:00pm	LUNCH
1:00pm	Adjourn of SAB

Afternoon Session: Argonne National Lab., Building 241

1:00 – 6:00pm	All-Hands Meeting on Codes (Room D-172)
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