Chemistry of Ice **New Orleans, LA**
Organizers: J. D. Cyran, J. D. Gezelter **March 17-21, 2024**

Sunday, March 17, 2024 | 8am – 12pm session
Ernest N. Morial Convention Center | Hall B, Rm. 4
Spectroscopy and Reactivity | J. Cyran, *Presiding*

8:00 AM. Introductory Remarks.

8:05 AM. Interfacial acid-base chemistry and the role of the hydrogen bonding network at the air-ice interface. **T. Bartels-Rausch**

8:35 AM. Photoionization dynamics of methane water and carbon dioxide clusters acting as proxies for astrochemically relevant ices. **N. Dias**, A. Lemmens, M. Ahmed

8:55 AM. Theoretical characterization of amorphous ices and carbonic acid clusters in the UV. **R.C. Fortenberry**

9:15 AM. Solute interactions governing reversible color loss of frozen organic dye solutions. **E. Asenath Smith**, D. Tague, T. Schutt, M.K. Shukla, G. Kosgei

9:45 AM. Intermission.

10:15 AM. Trapping heterogeneous NO_2 hydrolysis reaction intermediates on ice. **J. Maurais,** P Ayotte

10:35 AM. Headspace gas measurements of the partitioning of organic gases to warm ice surfaces. **R.R. Michelsen**, J. Charney, D. Teri, M. Askew, S. Reagle

11:05 AM. Modeling photochemical reactions at the air-ice interface. **D. Donadio**, M. Berrens, K. Chan, Z. Chen

11:25 AM. Investigations of gaseous condensation including isotope effects, gas capture, reactivity, adhesion and the nature of the quasi-liquid boundary layer of molecular ices. M. Brann, R.S. Thompson, K.D. Gibson, X. Ma, B. Hance, Y. Ma, **S.J. Sibener**

Sunday, March 17, 2024 | 2pm – 6pm session
Ernest N. Morial Convention Center | Hall B, Rm. 4
Structure and Inhibition | D. Donadio, *Presiding*

2:00 PM. Characterizing hydrogen-bonding interactions in cryoprotectant mixtures. **C. Baiz**

2:30 PM. Toward the rational design of novel cryoprotectants. M. Warren, F. Bachtiger, M.I. Gibson, **G.C. Sosso**

3:00 PM. Intermission.

3:50 PM. Ice growth and dynamics. **M.J. Shultz**, E. Gubbins

4:20 PM. Intermission.

4:40 PM. Realistic view of ice from data-driven many-body simulations. R. Rashmi, **F. Paesani**

5:10 PM. Formulation of the many-body expansion (MBE) for periodic systems: Application to ice. **K.M. Herman**, S.S. Xantheas

5:30 PM. Enabling large-scale condensed-phase hybrid density functional theory based *ab initio* molecular dynamics: Application to the ice I*h*-II-III triple point. **H. Ko**, J.A. Harris, B. Santra, R.A. Distasio

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Wednesday, March 20, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | R06
Bio-ice | S. Sarupria, *Presiding*

2:00 PM. Investigation of the ice nucleation properties of birch pollen. **E. Backus**, F. Strahl, C. Saak, M. Mezger, F. Reyzek, H. Grothe

2:30 PM. The most potent snow makers. **Y. Qiu**, V. Molinero, I. de Almeida Ribeiro

2:50 PM. E Pluribus Unum: Functional aggregation of cell-free proteins enables fungal ice nucleation. **K. Meister**

3:20 PM. Intermission.

3:40 PM. Structure-activity relationship of natural and engineered antifreeze proteins. Y. Shalom, E. Miller, **R. Drori**

4:10 PM. Molecular insights into the interactions between antifreeze proteins and ice. A. Thosar, Y. Cai, J. Choi, Z. Vicars, S. Marks, **A. Patel**

4:40 PM. Intermission.

5:00 PM. Exploring cryogenic dynamics in aqueous solutions: From ice nanocrystal formation to protein hydration. **F. Perakis**

5:30 PM. Ice-binding proteins up close and personal. **I. Voets**

Thursday, March 21, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R06
Surface Dynamics and Nucleation | G.C. Sosso, *Presiding*

8:00 AM. Atomistic simulations of molecule formation on amorphous solid water ices. **M. Meuwly**

8:30 AM. On slippery ice. L. Baran, P. Llombart, W. Rzysko, **L.G. MacDowell**

9:00 AM. Intermission.

9:15 AM. Structural and dynamic changes at ice/water interfaces in contact with small molecule cryoprotectants. **J.D. Gezelter**, B.M. Harless

9:45 AM. Symphony of interactions: Interfacial water, ions, and phase transitions. **S. Sarupria**

10:15 AM. Intermission.

10:30 AM. Progress in understanding ice nucleation with insights from water activity and substrate properties. **D.A. Knopf**, P.A. Alpert

11:00 AM. Heterogeneous nucleation of water under tension. **W.H. Cantrell**, E. Rosky, T. Li, I. Nakamura, R. Shaw

11:30 AM. The role of surface features in promoting heterogeneous ice nucleation. **M. Freedman**

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