

Liquid And Electrolyte Anomalies in Nano-Confinement: Structure, Dynamics, and Reactivity

Organizers: *Marialore Sulpizi, Anastasia Ilgen, Louise Criscenti, Kevin Leung*

New Orleans, LA

March 18-21, 2024

Monday, March 18, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R08

Electric Double Layer Structure | M. Sulpizi, *Presiding*

8:00 AM. Structure and dynamics of electric double layer. **M. Toney**

8:30 AM. Advances in the simulation of electrified Interface at the nanoscale. **C. Cucinotta**

9:00 AM. Water-DMSO cosolvent mixtures to control hydrogen-bonding at a gold electrode interface. **Z. Al-Mualem, K. Lorenz-Ochoa,** L. Pan, H. Ren, C. Baiz

9:15 AM. Application of charge regulation to measurements of pH in the vicinity of a silica surface. **J. Lutzenkirchen,** F. Heberling

9:45 AM. Studying electric field fluctuations in electrode-electrolyte systems using molecular dynamics simulations. **J. Nauman,** A. Willard

10:00 AM. Intermission.

10:10 AM. Controlling electric fields and hydration at the junctions between surfactants and metals. **J. Dawlaty**

10:25 AM. Strong anisotropic electronic coupling between gold surfaces and interfacial water. **C. Park,** B. Das, D. Marx

10:55 AM. Molecular insights in mineral-water interfaces with sum frequency generation spectroscopy. **E. Backus,** M. Zelenka

11:25 AM. Surface specific vibrational Spectroscopy of angstrom-scale confined water. **M. Bonn,** Y. Wang, Y. Nagata

Monday, March 18, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | R08

Nanoconfinement: Effects on Water Structure and Dielectric Properties | K. Leung, M. Sulpizi, *Presiding*

2:00 PM. Dielectric and spectroscopic properties of ions and water in nano-confinement. **R. Netz**

2:30 PM. Unravelling the anomalous dielectric properties of interfacial and strongly confined water. **I. Fumagalli**

3:00 PM. Finding infinities in nanoconfined geothermal electrolyte static dielectric properties, and implications on ion adsorption/pairing. **K. Leung**

3:15 PM. Modeling ionic correlations and dielectric response in nanoconfined liquids. **R.C. Remsing**

3:30 PM. Radiolysis of water confined in aluminosilicate nanotubes: Importance of charge separation effects. **S. Le Caer**

4:00 PM. Intermission.

4:10 PM. Modeling the structure and dynamics of nanoconfined fluids. **J.A. Greathouse**

4:40 PM. Spectroscopy and dynamics of water-silica interfaces. H.S. Senanayake, J.A. Greathouse, **W.H. Thompson**

5:10 PM. On De Gennes Narrowing of Fluids Confined in Nanoporous Materials. Wanda Kellouai, Jean-Louis Barrat, Patrick Judeinstein, Marie Plazanet, **Benoit Coasne**

5:40 PM. Polarizable model of graphite and its applications to nanotechnology. **K. Kanhaiya,** J. Winetrou, M. Sulpizi, H. Heinz

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Wednesday, March 20, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R07

Nanoconfined Water; Dissolution, Nucleation and Precipitation in Nanopores

L. J. Criscenti, K. Leung, *Presiding*

8:00 AM. Introductory Remarks.

8:05 AM. Surface passivation during carbonation under low water supercritical carbon dioxide. **J. Loring**, B. Rajan, S.D. Burton, G.M. Bowers, M. Bowden, O. Qafoku, C.J. Thompson, S.N. Kerisit, S.T. Mergelsberg

8:35 AM. Structure, dynamics, and reactivity of liquid water in single-digit nanopores from machine learning molecular simulations. **T. Pham**

9:05 AM. Vibrational intensity anomalies upon nano-confinement. **E. Borguet**

9:35 AM. Confinement-induced clustering of H₂ and CO₂ gas molecules in hydrated clay interlayer. **A. Choudhary**, T.A. Ho

9:50 AM. Intermission.

10:05 AM. Nucleation of amorphous phases under nano-confinement. **A.G. Stack**, H. Wang, K. Yuan, J. Weber, V. Starchenko, S.A. Chen, T. Liu

10:35 AM. Effect of confined water on oriented attachment of gibbsite nanoparticles. **T.A. Ho**

11:05 AM. Accelerated oligomer formation of pyruvic acid in submicron aerosols. **P. Kim**, R.S. Reynolds, M. Ahmed, K.R. Wilson

11:20 AM. How calcite dissolution is inhibited by dissolved Pb²⁺ in confined fluids. B. Abdilla, S. Lee, N.C. Sturchio, **P. Fenter**

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

Ernest N. Morial Convention Center | R09

Nanoconfinement: Surface Chemistry Effects and Acidity | L. J. Criscenti, A. G. Ilgen, *Presiding*

2:00 PM. Introductory Remarks.

2:05 PM. Exploring confinement effects in electrochemistry by single entity and spectro-electrochemistry. **C. Bondü**

2:35 PM. How confinement impacts osmolytes and how osmolytes affect confining environments. **N.E. Levinger**, B.L. Gourley, G. Virgen, M. Halliday, H. Afzal, T. Nguyen

3:05 PM. Aqueous chemistry in nanopores with chemical functional groups. **Y. Jun**, Y. Zhu, P. Gupta, H. Derami, S. Singamaneni

3:35 PM. Treatment of buried charges and confined water in protein cavities: Electronic polarization and grand canonical Monte Carlo sampling. **J. Deng**, Q. Cui

3:50 PM. Confinement and interfaces make water weird: Observations with ultra-sensitive magnetic resonance cross-relaxation. **J. Franck**

4:05 PM. Intermission.

4:20 PM. Quantum plumbing: Towards the quantum control of nanoscale flows. **N. Kavokine**

4:50 PM. Experimental study of viscosity of liquids at low Reynolds number. **W. K Bani**

5:05 PM. Unveiling the roles of nanoconfined water in enhancing interfacial reactions. **T. Tang**, W. Ding, X. Zhang

5:20 PM. Temperature dependence of secondary chemistry in the ozonolysis of unsaturated organic aerosol. **R.S. Reynolds**, K.R. Wilson

5:35 PM. Proton dissociation and delocalization in hydrated acidic zeolites. **J. Hack**, X. Ma, Y. Chen, N. Lewis, H. Kung, G.A. Voth, A. Tokmakoff

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

Ernest N. Morial Convention Center | R09

Interfacial Reactions in Nanopores | L. J. Criscenti, A. G. Ilgen, *Presiding*

8:00 AM. Introductory Remarks.

8:05 AM. Visualization of ion-to-surface binding, binding energy quantification, and charge regulation in confined geometries. F. Altmann, J. Lee, U. Ramach, M. Olgiati, L. Mears, A. Celebi, J. Dziadkowiec, D. Lee, **M. Valtiner**

8:35 AM. Iontronics - Ionic selectivity under angstrom-scale confinement. **R. Boya**

9:05 AM. Adsorption kinetics of lanthanides in silica nanopores. **B.T. Fashina**, J. Smith, A.G. Ilgen

9:20 AM. Effect of the environment on acid-base chemistry within nanopores. **A. Baldo**, A.G. Ilgen, K. Leung

9:35 AM. The thermodynamics of ion exchange and adsorption reactions in nano-confinement. **N. Kabengi**, A.G. Ilgen

10:05 AM. Intermission.

10:20 AM. High-frequency dynamics of water and ions in Clay interlayer nanopores. **I.C. Bourg**, T.R. Underwood

10:50 AM. Separating nickel and cobalt in aqueous solutions using reactive nanopores in functionalized MOF-808 metal-organic frameworks. **B. Song**, R.E. Sikma, D.F. Sava Gallis, A.G. Ilgen

11:05 AM. Quantifying the effects of dissolved nitrogen and carbon dioxide on drying pressure of hydrophobic nanopores. **H. Binyaminov**, J. Elliott

11:20 AM. Hydrogen bond energetics and deprotonation of organic acids in silica nanopores. **A.G. Ilgen**