

Sunday, March 17, 2024 | 8am – 12pm session

Ernest N. Morial Convention Center | R08

D. G. Kuroda, *Presiding*

8:00 AM. Introductory Remarks.

8:10 AM. Vibrational dynamics in ionic liquid composite materials. **S. Garrett-Roe**

8:40 AM. Preferential solvation dynamics in ternary solutions probed with 2D-IR spectroscopy. V.F. Crum, **K.J. Kubarych**

9:10 AM. Water in MOFs: Vibrational insights into confinement, adsorption, and molecular interactions. C. Ho, H. Frank, **F. Paesani**

9:30 AM Intermission.

9:50 AM. Long-range interfacial effects in room temperature ionic liquid thin films. **M.D. Fayer**, j.P. Breen, I.C. Leibfried, X. Xing

10:20 AM. 2DIR reveals ion dependent spectral diffusion in precisely controlled polymeric membranes. **R. Ball**, C. Johnson, L. Zhang, s. oh, A. Patel, K.I. Winey, C.O. Osuji, J.M. Anna

10:35 AM. Probing the dynamics of inorganic ligand-quantum dot interactions: Insights from 2D IR spectroscopy. **S. Bagchi**

11:05 AM. IR absorption and NMR spectroscopy: Combining the very fast and the very slow in order to map the hydration shell structure of the proton one molecule at a time. D. Pines, E. Kozari, **E. Pines**

11:25 AM. Structure and dynamics of mixed salts in poly(ethylene glycol) diacrylate. **E. Alasadi**, C. Baiz, E. Zofchak

Sunday, March 17, 2024 | 2pm – 6pm session

Ernest N. Morial Convention Center | R05

D. G. Kuroda, *Presiding*

2:00 PM. Ultrafast dynamics of phonon polaritons after electronic excitation. **A.D. Dunkelberger**, C.T. Ellis, D.C. Ratchford, D.S. Katzer, V.M. Breslin, T.J. Michael, M. Kim, C. Kim, I. Vurgaftman, J. Tischler, J. Caldwell, J. Owrutsky

2:30 PM. Combining physics-based and data-driven models for accelerating condensed phase spectroscopy simulations. **D.P. Tabor**

3:00 PM. Measuring depth-dependent rigidity and fluidity of lipid bilayer interior with vibrational spectroscopies. M. Islam, S.U. Nawagamuwage, **I.V. Rubtsov**

3:30 PM. Real-time mapping of transient electric dipole moments by terahertz Stark spectroscopy. **P. Singh**, J. Zhang, D. Engel, B.P. Fingerhut, M. Broser, P. Hegemann, T. Elsaesser

3:45 PM. Advancing infrared reflection absorption spectroscopy for single atom catalysts on metal oxide supports. **J. Pavelec**, D. Rath, M. Eder, M. Schmid, U. Diebold, G.S. Parkinson

4:00 PM. Intermission.

4:20 PM. Modeling thermal transport in molecules. **D. Leitner**

4:50 PM. Characterization of thermal energy transport in heated nanostructures using inelastic scattering of focused electron beams. **G. Duddy**, E.K. Beutler, V. Kumar, M.R. Bourgeois, J. Hachtel, D.J. Masiello, J.P. Camden

5:05 PM. Application of 2D IR to investigate the structure and dynamics of highly scattering-producing samples. **Y.S. Kim**

5:35 PM. Finite temperature effects on vibronic spectra from the variational thermo-field Gaussian wavepacket dynamics. **R. Moghaddasi Fereidani**, Z. Tong Zhang, J. Vanicek

Tuesday, March 19, 2024 | 2pm – 6pm session
Ernest N. Morial Convention Center | Hall B, Room 4
A. Ghosh, *Presiding*

2:00 PM. Resolution limits and heat dissipation in photothermal microscopy. J. Bhandari, B. Brown, J. Huffman, J. Jodway, **G.V. Hartland**

2:30 PM. Vibrational exciton nano-crystallography: A molecular ruler to image structure, coupling, and disorder in functional materials. **M.B. Raschke**

3:00 PM. Imaging the graphene quantum electron motion in real time and space. D. Hui, H. Alqattan, M. Sennary, N. Golubev, **M. Hassan**

3:20 PM. Exploring chemical dynamics in solution using fluorescence-encoded infrared spectroscopy. **S. Lee**, L. Whaley-Mayda, A. Guha, A. Tokmakoff

3:35 PM. Spatially resolved photothermal infrared spectroscopy of antiparallel amyloid aggregates in cerebral amyloid angiopathy. **A. Ghosh**

3:55 PM. Intermission.

4:15 PM. Stimulated Raman photothermal microscopy. **J. Cheng**

4:45 PM. Functional bond-selective microscopy for subcellular bioanalysis. **L. Wei**

5:15 PM. Applying anharmonic localized normal mode DVR calculations to the Raman spectroscopy of terminal alkynes. **C.A. Daly**, K. Streu, A. Aneesh, J. Patel, T. Haupt

5:45 PM. Surface-enhanced Raman spectroscopy and deep learning for bacterial wastewater monitoring. **L.K. Herndon**, B. Ogunlade, Y. Zhang, S. Dagli, H. Balch, F. Safir, A. Boehm, J. Dionne

Wednesday, March 20, 2024 | 8am – 12pm session
Ernest N. Morial Convention Center | Hall B, Room 4
A. Ghosh, *Presiding*

8:00 AM. Absolute stimulated Raman cross sections: A unified framework of molecular response. **W. Min**

8:30 AM. Detecting Interplay of chirality, water, and interfaces for elucidating biological functions. **E.C. Yan**

9:00 AM. Rapid infrared spectroscopic imaging for zebrafish development toxicology dynamics. **R. Bhargava**, M.P. Confer, K. Yeh, K. Falahkeirkhah, I. Lebovic, A. Bhargava, W. Mei

9:30 AM. Dynamics of the acoustic vibrations of gold nanoplates. **C. Wright**, G.V. Hartland

9:45 AM. Applying infrared spectroscopy to characterise the structure and form of pharmaceutical cocrystals. **R.S. Dosanjh**, D. Lennon, S.F. Parker, A. York

10:00 AM. Intermission.

10:20 AM. Distinguishing spectator from driving modes in photoinduced chemical reactions. **R.R. Frontiera**

10:50 AM. A reliable and simple computational method for the characterization of complex molecular systems using IR spectroscopy, **L. X. Sepulveda**, J. F. Galindo, D. G. Kuroda

11:05 AM. Second-order spectral lineshapes from charged interfaces. **F. Geiger**

11:35 AM. Terahertz spectroscopy as a validation tool for pharmaceutical crystal structure prediction. **S. Zarrella**, M. Mohara, K. Shimura, T.M. Korter

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

Ernest N. Morial Convention Center | Hall B, Room 4

M. J. Tucker, *Presiding*

2:00 PM. Vibrational dynamics under an applied field at the surface of an electrode using 2D IR spectroscopy. **M.T. Zanni**

2:30 PM. Time-resolved *in situ* electrochemical SFG study of hot electron transfer from metal electrodes to adsorbates. **T. Lian**

3:00 PM. Ion pairing in Aqueous electrolytes. **S. Corcelli**

3:30 PM. Ultrafast transient and two-dimensional infrared spectroscopies of isolated, cryogenically cooled molecular ions. Z. Ma, L. Chen, **J.A. Fournier**

3:55 PM. Intermission.

4:10 PM. THz collective modes gate liquid dynamics. **M.T. Cicerone**

4:40 PM. Vibrationally probing the making and breaking of Lewis bonds at interfaces: Odd potential dependence and ultraslow dynamics. **J. Dawlaty**

5:10 PM. Forecasting absorption profiles of electrochromic polymers from neutral to doped states. **J. CHAUDHARY, Z. Wang, L.V. Slipchenko, J. Mei**

5:25 PM. Binding-induced lipid domains: Peptide-membrane interactions with pip₂ and PS. **X. Chen, Z. Al-Mualem, A. Shafieenezhad, E. Senning, C. Baiz**

5:40 PM. Uncovering Water-Dependent Behaviors in Ionic Liquid Electrolytes with 2D IR Spectroscopy & Imaging. **A.T. Krummel, C. Tibbetts, B. Luther**

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

Ernest N. Morial Convention Center | Room 232

M. J. Tucker, *Presiding*

8:00 AM. Structural insights into amyloidogenic Tau hexapeptide PHF6: A 2DIR study. **A.L. Serrano**

8:30 AM. Investigating peptide structure and polymorphism with 2D IR spectroscopy and transition dipole strength analysis. **L.E. Buchanan**

9:00 AM. Combining variable temperature infrared spectroscopy and unique nucleobase isotope editing methods to gain sub-molecular insights into nucleic acid structural stability: Calibrating a molecular thermometer to measure local base pair melting. **A.L. Stelling**

9:30 AM. Elucidating ion configurations and water dynamics in a K⁺ ion channel using two-dimensional infrared spectroscopy. **A.A. Kananenka, M.J. Ryan, L. Gao, F. Valiyaveetil, M.T. Zanni**

9:50 AM. Intermission.

10:30 AM. Isotope labeling without the pain: A microsampling approach to monitoring protein structure in cell and in solution. J.H. Wat, **M. Reppert**

11:00 AM. Probing photosystem I, model systems, and photocatalysts with mixed vibrational and electronic spectroscopies. **J.M. Anna**

11:30 AM. Probing vibrational energy transfer in complex ligand scaffolds with 2D IR spectroscopy. **C. Mallon, M. Zafar Abbas, A. de Bettencourt-Dias, M.J. Tucker**

11:45 AM. Charge identity perturbs dynamics Inside Biocondensates. **K. Lorenz-Ochoa, C. Baiz**

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