

# Electric Field Effects in Vibrational Spectroscopy

Organizers: Bogdan Dereka and Alexei Kananenka

March 22-24, 2026

## Sunday AM

Georgia World Congress Center | B310

### **Infrared and THz Stark Spectroscopy**

B. Dereka, A. A. Kananenka, *Organizers* | N. Lewis, *Presiding*

**8:00 AM.** Introduction and opening remarks.

**8:05 AM.** Vibrational Stark spectroscopy: Fundamentals and applications. **S.G. Boxer**

**8:50 AM.** Electrostatic characterization of non-covalent interactions built in metal-organic frameworks. **Z. Ji**

**9:10 AM.** Stark effect in the determination of pocket sizes in polymers and ionic liquids. M.D. Fayer, J. Pan, **A. Charnay**, L. Leibfried

**9:55 AM.** Intermission.

**10:15 AM.** Electric interactions in liquids and proteins mapped by ultrafast terahertz methods. **T. Elsaesser**

**11:00 AM.** Computational study of alkyne C–H vibrational shifts in the terahertz regime: hydrogen bonding and local electric fields. **A. Biswas**, B. Dereka, A.A. Kananenka

**11:15 AM.** Local thermodynamics and electric fields at an electrified interface. **N. Strasser**, M. Havenith

# Electric Field Effects in Vibrational Spectroscopy

Organizers: Bogdan Dereka and Alexei Kananenka

March 22-24, 2026

## Sunday PM

Georgia World Congress Center | B310

### Theory & Water

B. Dereka, A. A. Kananenka, *Organizers* | Z. Ji, *Presiding*

**2:00 PM.** Technical remarks.

**2:05 PM.** On the electric double layer at air-aqueous electrolyte interfaces: a machine learning molecular dynamics study of structure and vibrational sum-frequency generation spectroscopy. I. Mezghani, M. de la Puente, **D. Laage**

**2:50 PM.** From neutral to charged graphene: how electric fields govern interfacial water. R. Rashmi, **F. Paesani**

**3:35 PM.** Stark spectroscopy from MD using advanced and machine-learned energy functions. **M. Meuwly**

**3:55 PM.** Intermission.

**4:15 PM.** Water at the edge: on-water Raman spectroscopy, electrostatics and chemistry. **W. Min**

**5:00 PM.** In the heart of CH: spectroscopic insights into proper C–H hydrogen bonds. **A. Kliuchynskyi**, A. Biswas, A. Shalit, A.A. Kananenka, B. Dereka

**5:15 PM.** Spectroscopic signatures of electric fields for chemical reactivity at soft interfaces. **T.L. Head-Gordon**

# Electric Field Effects in Vibrational Spectroscopy

Organizers: Bogdan Dereka and Alexei Kananenka

March 22-24, 2026

## Monday AM

Georgia World Congress Center | B310

### **Complexity of Electrochemical Interfaces**

B. Dereka, A. A. Kananenka, *Organizers* | A. Wuttig, *Presiding*

**8:00 AM.** Technical remarks.

**8:05 AM.** Connecting interfacial field, electrode-induction and hot electron transfer.

**T. Lian**

**8:50 AM.** Electric fields at electrochemical interfaces: vibrational probes and electrocatalysis. **S. Hammes-Schiffer**

**9:35 AM.** Complexities in vibrational electrochromism of monolayers for studying interfacial solvation. A. Pennathur, R. Kumawat, G.C. Schatz, A. Tokmakoff, **N. Lewis**

**10:20 AM.** Intermission.

**10:40 AM.** Structural dynamics under an applied voltage: 2D IR spectroscopy of electrode interface. **M.T. Zanni**

**11:25 AM.** Fractional charge density functional theory for predicting vibrational frequencies, bond strengths, and acid-base equilibria at electrochemical interfaces.

**J. Kim, W. Yang**

**11:40 AM.** Modulating interfacial hydrogen-bond networks using cosolvents and electrode potential. **C. Baiz**

# Electric Field Effects in Vibrational Spectroscopy

Organizers: Bogdan Dereka and Alexei Kananenka

March 22-24, 2026

## Tuesday AM

Georgia World Congress Center | B310

### **Effects of Electric Fields and Ions on Chemical Reactivity and Catalysis**

B. Dereka, A. A. Kananenka, *Organizers* | J. M. Gibbs, *Presiding*

**8:00 AM.** Technical remarks.

**8:05 AM.** Taking charge of local electric fields and hydration: crowns, soaps, interfaces.  
**J. Dawlaty**

**8:50 AM.** Examining the electric double layer structure during CO<sub>2</sub>-to-CO conversion with vibrational Stark spectroscopy. **M. Waegele**

**9:35 AM.** Characterizing interfacial and bulk structure of electrocatalysts with vibrational spectroscopy. **A. Wuttig**

**10:20 AM.** Intermission.

**10:40 AM.** Ultrafast vibrational dynamics in electrolyte solutions. V.F. Crum, A. Mon, A. Mohammadi, **K.J. Kubarych**

**11:25 AM.** Decoding spectral shape variability in SERS: integrating substrate, orientation, and ai-based analysis. **A. Kumar**, F. Ma, X. Chen, Y. Zhao

**11:40 AM.** Theoretical insights into the resonant suppression effect in vibrational polariton chemistry. **P. Huo**

# Electric Field Effects in Vibrational Spectroscopy

Organizers: Bogdan Dereka and Alexei Kananenka

March 22-24, 2026

## Tuesday PM

Georgia World Congress Center | B310

### **Oxide Interfaces, Biological Systems**

B. Dereka, A. A. Kananenka, *Organizers* | M. Waegele, *Presiding*

**2:00 PM.** Second-order vibrational lineshapes from charged interfaces. **F. Geiger**

**2:45 PM.** Horizontal and vertical water ordering at aqueous oxide interfaces and their SFG vibrational signatures. **M.P. Gaigeot**

**3:05 PM.** pH evolution of the electrical double layer at charged oxide/electrolyte interfaces. **J.M. Gibbs**

**3:50 PM.** *In situ* characterization of reactive complex-containing self-assembled monolayers under applied E-fields using sum frequency generation. C. Egemba, H. Haq, E. Hill, **P.E. Ohno**

**4:10 PM.** Intermission.

**4:30 PM.** Electrostatics and dynamics in complex lipid bilayer membranes. **L.J. Webb**

**4:50 PM.** Two vibrational probes with complementary solvatochromism report on carrier protein substrate sequestration with minimal perturbation. **C.H. Londergan**, A. Marmer, G. Patel, K. McDonnell, L.K. Charkoudian

**5:10 PM.** Local environment influence ON mid-infrared photothermal contrast. **L. Biondelli**, E. Podshivaylov, Y. Ding, W. Stradley, U. Filippi, P. Frantsuzov, M.K. Kuno

**5:25 PM.** Development of spectroscopic maps for terminal alkyne containing molecules to explain raman spectra. **C.A. Daly**, A. Aneesh, K. Streu, E. Song, T. Haupt

**5:45 PM.** Concluding remarks and closing.

*A special thanks to our sponsors for their generous support:*

