

Physical Chemistry of Molecular Electronics

Organizers: Maria Kamenetska, Tim Su, Gemma C. Solomon, Michael S. Inkpen, Zhenfei Liu, Ryan C. Chiechi

New Orleans, LA

March 17-18, 2024

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

Ernest N. Morial Convention Center | R05

New Molecular Paradigms for Molecular Electronics | M. Kamenetska, *Presiding*

8:00 AM. Porphyrin-based molecular wires and nanorings. **H. Anderson**

8:25 AM. Lewis-acid mediated reactivity in single-molecule junctions. **J. Prana**, L. Kim, G. Homann, M.S. Inkpen

8:40 AM. Electron transport in heme-containing peptide monolayers for biohybrid molecular electronics. **H. Yang**, X. LIU, L. Zhang, M. Meigooni, J. Ren, E. Tajkhorshid, M.D. Losego, J.S. Moore, C. Schroeder

8:55 AM. Intermission.

9:10 AM. Charge transport in single carbon nanorings and nanobelts. **Y. Zang**

9:35 AM. Exploring charge transfer and transport in osmium(IV) tetraaryl complexes. **L. Zagami**, M.S. Inkpen

9:50 AM. Flicker noise analysis of single molecule break junction data shows complex oligoynes molecular wire features. **J.M. Morris**, J. Potter, S.J. Higgins, R. Nichols, P. Low, A. Vezzoli

10:05 AM. Single-molecule junction studies using low vapor pressure solvents. K. Nguyen, L. Kim, S. Stuke, T.M. Czyszczon-Burton, J. Prana, Z. Miao, S. Park, **M.S. Inkpen**

10:20 AM. Intermission.

11:00 AM. (VIRTUAL TALK) Mechanosensitive Molecular Switches. **S. Sangtarash**

11:25 AM. Structure-conductance relationships in single molecule junctions from density-functional theory calculations of thousands of junction geometries. **H. Vazquez**

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

Ernest N. Morial Convention Center | R08

Conductance Switching and Functionality | Z. Liu, *Presiding*

2:00 PM. Dynamic molecular switches with hysteretic negative differential conductance emulating synaptic behavior. **E. del Barco**, W. Yulong, Q. Zhang, H. Astier, C. Nickle, A. Fuad, S. Saurabh, A. Borrini, Z. Zhang, C. Honnigfort, B. Braunschweig, a. leoncini, D. Qi, D. Thompson, C. Nijhuis

2:25 PM. Photooxidation driven formation of Fe-Au linked ferrocene-based single-molecule junctions. **W. Lee**, L. Li, M. Camarasa-Gómez, D. Hernangómez-Pérez, X. Roy, F. Evers, M.S. Inkpen, L. Venkataraman

2:40 PM. Molecular memristors based on interlocked supramolecules. **Yu Xie**, Yuan Li

3:10 PM. Multifunctional molecular electronic devices. **Y. Li**

3:35 PM. Intramolecular London dispersion interactions in single-molecule junctions. **M.O. Hight**, J. Wong, A.E. Pimentel, T.A. Su

3:50 PM. Giant rectification in molecular diode induced by structural evolution under electric field. **J. Lin**, Y. Li

4:05 PM. Intermission.

4:20 PM. Correlation between conformational analysis and molecular electronics. **M.M. Thuo**, J. Chen, C. Du

4:45 PM. New silver contact chemistries in single-molecule junctions. **T.M. Czyszczon-Burton**, E. Montes, H. Vazquez, M.S. Inkpen

5:00 PM. Bending bands and hybridizing interfaces on Si(111) substrates: Electronic benefits for photoelectrochemistry. **M.J. Rose**

5:25 PM. Ladder-type molecules for robust and switchable molecular electronic devices. **C. Schroeder**

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

Radicals and Topological Insulator Behavior | M. S. Inkpen, *Presiding*

8:00 AM. Ultrahigh conductance in radical based long molecular wires. **L. Venkataraman**

8:25 AM. Dynamical screening of the local spin moments at metal-molecule spintronic interfaces. S. Bhandary, E. Poli, G. Teobaldi, **D. O'Regan**

8:40 AM. Highly-oxidised indolocarbazoles: Open-shell candidates for single-molecule electronics. **M. Gatto**, A. Vezzoli, C. Liu

8:55 AM. Intermission.

9:10 AM. From Semiconductors to metals: Engineering topological states in nanographenes. **F.R. Fischer**

9:35 AM. Quantifying the role of intermolecular interactions on tunneling transport in molecular junctions. **G. Jeong**, C.D. Frisbie

9:50 AM. From Liouville to Landauer: A scattering approach to tunneling and hopping transport. **R. Jorn**, D. Bialas

10:05 AM. Intermission.

10:20 AM. Topological insulator single molecule circuits formed with neutral organic radicals. **M. Kamenetska**

10:45 AM. Active space methods for characterizing conductance decay reversals in molecular electronics. **E.P. Hoy**

11:00 AM. Highly efficient long-range quantum transport in single open-shell conjugated oligomers. **K. Wang**, C. Tang, M. Shiri, N. Eedugurala, J. Azoulay, I. Franco - **WITHDRAWN**

11:25 AM. Electronic and steric stabilisation of single-radicaloids junctions. **A. Vezzoli**, A. SIL, R. Nichols, M.F. Gatto, C. Liu, J.M. Morris

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

Ernest N. Morial Convention Center | R09

Chirality-Induced Spin Selectivity (CISS) and Quantum Interference (QI) | R. C. Chiechi, *Presiding*

2:00 PM. Spin-polarized charge transmission enabled by highly conjugated chiral structures. **M.J. Therien**

2:25 PM. Enhanced chemical gating in single-molecule junctions by Fano resonance. **W. Shi**, C.R. Prindle, L. Li, J. Jessen, B. Laursen, M.L. Steigerwald, C.P. Nuckolls, L. Venkataraman

2:40 PM. Orthogonal Spiropyran-Based Molecular Wires for Well-Defined Electrosteric Switching. **L. Chongguang**, A. Vezzoli

2:55PM. Intermission.

3:10 PM. (VIRTUAL TALK) Room-temperature constructive quantum interference from single organometallic molecules to self-assembled molecular-electronic films. **N.J. Long**

3:35 PM. Many-body coherence in molecular electronics. **L. Hsu**, C. Hang

3:50 PM. Nonadiabatic nuclear dynamics with strong light-matter interactions in quantum transport: Floquet frictional effects, Lorentz-like forces, and spin selectivity. **J. Chen**, W. Liu, V. Mosallanejad, W. Dou

4:05 PM. Intermission.

4:20 PM. Experimental studies into the nature of spin-dependent electronic processes of chiral molecules. **D.H. Waldeck**

4:45 PM. Quantum interference in saturated tetrel clusters. **A. Pimentel**, M.O. Hight, T. Siu, M. Aguirre Cardenas, T.A. Su

5:00 PM. (VIRTUAL TALK) Electrical properties of SARS-CoV-2 spike proteins. **N. Darwish**

5:25 PM. (VIRTUAL TALK) Spin interference for molecular electronics. **H. Sadeghi**

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