



Telluride Science Research Center

**Organizers:** Daniel Kosov and Michael Thoss

**TSRC Hosts:** Nana Naisbitt 970-708-0004 and Rory Sullivan 970-708-4542

**Location:** Telluride Intermediate School, 725 West Colorado Ave

	Monday	Tuesday	Wednesday	Thursday	Friday
8:00 am	Breakfast	Breakfast	Breakfast	Breakfast	Breakfast
8:30 am					
9:00 am	R. Nichols 8:40-9:35	S. Higgins 8:30-9:10	free	L. Venkataraman 8:30-9:10	Group hike
9:30 am		M. Thoss 9:10-9:50		B. Dunietz 9:10-9:50	
10:00 am	A. Nitzan 9:35-10:30	G. Solomon 9:50-10:30		C. Herrmann 9:50-10:30	
10:30 am	Coffee Break	Coffee Break		Coffee Break	
11:00 am	G. Kirzenow 10:50-11:30	J. Hihath 10:50-11:30		V. Mujica 10:50-11:30	
11:30 am	F. von Oppen 11:30-12:10	J. Neaton 11:30-12:10	J. Reimers 11:30-12:10		
12:00 am					
12:30 am					
1:00 pm					
1:30 pm					
2:00 pm			H. van der Zant 13:30-14:10		
2:30 pm	P. Reddy 14:00-14:40	U. Peskin 14:00-14:40	M. Hybertsen 14:10-14:50	O. Tal 14:00-14:40	
3:00 pm	C. Stafford 14:40-15:20	O. Hod 14:40-15:20	F. Evers 14:50-15:30	Y. Selzer 14:40-15:20	
3:30 pm	Coffee Break	Coffee Break	Coffee Break	T. Novotny 15:20-16:00	
4:00 pm	H. Wang 15:40-16:20	D. Natelson 15:40-16:20	E. Rabani 15:50-16:30	Coffee Break	
4:30 pm	M. Galperin 16:20-17:00	T. Frederiksen 16:20-17:00	D. Segal 16:30-17:10	F. Grozema 16:20-17:00	
5:00 pm					
5:30 pm			M. Wegewijs 17:10-17:50	M. Ratner 17:00-17:55	
6:00 pm					
6:30 pm		TSRC Town Talk 18:00-19:15	Picnic BBQ 18:00-21:00 Ah Haa School for the Arts 300 S. Townsend		
7:00 pm		Historic Opera House 110 N. Oak Street			
7:30 pm					
8:00 pm					

## Monday

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8:30–8:40                      Opening

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Morning Session

Chair: Mark Hybertsen

8:40–9:35    Richard Nichols    Electrochemistry and single molecule electronics (+  
Overview)

9:35–10:30    Abraham Nitzan    Spin selectivity in electron transmission through chiral  
molecular layers (+ Overview)

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10:30–10:50                      Coffee Break

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10:50–11:30    George Kirczenow    Getting to know a molecular wire

11:30–12:10    Felix von Oppen    Adiabatic quantum motors

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Afternoon Session

Chair: Tomas Novotny

14:00–14:40    Pramod Sangi Reddy    Heat dissipation in atomic-scale junctions

14:40–15:20    Charles Stafford    Probing Maxwell's Demon with a nanoscale ther-  
mometer

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15:20–15:40                      Coffee Break

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15:40–16:20    Haobin Wang    Correlated quantum transport through model junc-  
tions

16:20–17:00    Michael Galperin    Charge and energy transport in molecular junctions

## Tuesday

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Morning Session		Chair: Doug Natelson
8:30–9:10	Simon Higgins	Anomalously low beta-values for 1,4-HS(CH <sub>2</sub> ) <sub>n</sub> -C <sub>6</sub> H <sub>4</sub> -(CH <sub>2</sub> ) <sub>n</sub> SH and some related terthiophene molecules; what is the conductance mechanism?
9:10–9:50	Michael Thoss	Charge transport in molecular junctions: Vibrationally induced decoherence, time-dependent transport, and graphene contacts
9:50–10:30	Gemma Solomon	Interference effects for electronics and thermoelectrics: Beyond mean-field and coherent tunneling
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10:30–10:50		Coffee Break
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10:50–11:30	Josh Hihath	Effects of molecule-electrode coupling on molecular transport
11:30–12:10	Jeffrey Neaton	Transport and level alignment in molecular junctions: Conductance, thermopower, and environmental effects
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Afternoon Session		Chair: Charles Stafford
14:00–14:40	Uri Peskin	Classical currents from transient coherences in molecular junctions
14:40–15:20	Oded Hod	A state representation approach for atomistic time-dependent transport calculations in molecular junctions
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15:20–15:40		Coffee Break
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15:40–16:20	Doug Natelson	Heating and voltage-tuning of molecular mechanical properties in nanoscale junctions
16:20–17:00	Thomas Frederiksen	DFT+NEGF simulations of transport phenomena in single-molecule junctions

## Wednesday

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Afternoon Session

Chair: Jeffrey Reimers

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|-------------|--------------------|---|
| 13:30–14:10 | Herre van der Zant | A statistical approach to measure single-molecule current-voltage characteristics                   |
| 14:10–14:50 | Mark Hybertsen     | Single molecule junctions: A laboratory for chemistry, mechanics and bond rupture                   |
| 14:50–15:30 | Ferdinand Evers    | Density of states in graphene with vacancies: Index theorems, runaway flow and frozen wavefunctions |

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15:30–15:50

Coffee Break

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|-------------|------------------|---|
| 15:50–16:30 | Eran Rabani      | Numerically exact reduced methods for nonequilibrium quantum impurity models  |
| 16:30–17:10 | Dvira Segal      | Path integral simulations of transport and dissipation: Vibrational instability in molecular rectifiers                     |
| 17:10–17:50 | Maarten Wegewijs | New developments in real-time Liouville-space transport theory: quantum field superoperators, fermion parity, and causality |

## Thursday

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### Morning Session

Chair: Herre van der Zant

- 8:30–9:10 Latha Venkataraman Electronics and mechanics of single molecule circuits
- 9:10–9:50 Barry Dunietz On thermoelectric properties of molecular junctions, thermal spin filtering and ghost bustering
- 9:50–10:30 Carmen Herrmann Electronic communication through molecular bridges

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10:30–10:50

Coffee Break

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- 10:50–11:30 Vladimiro Mujica Anomalous long-distance electron transfer and the role of chirality-induced spin polarization
- 11:30–12:10 Jeffrey Reimers Challenges for the accurate simulation of anisotropic charge mobilities through organic molecular crystals: The phase of mer-tris(8-hydroxyquinolato)aluminum(III) (Alq3) crystal

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### Afternoon Session

Chair: Ferdinand Evers

- 14:00–14:40 Oren Tal Relating atomic scale conductance to orbital structure by shot noise measurements
- 14:40–15:20 Yoram Selzer Measurement of large current noise in molecular junctions with a redox center
- 15:20–16:00 Tomas Novotny Various aspects of IETS calculations in nanoscopic systems

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16:00–16:20

Coffee Break

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- 16:20–17:00 Ferdinand Grozema Charge transfer in cross-conjugated systems: Connecting chemistry and physics
- 17:00–17:55 Mark Ratner Three short stories: An Ehrenfest adventure, real-time interference, and acid/base issues (+ Overview)
- 17:55–18:00 Closure