



Quantum Transport in Nanoscale Molecular Systems

July 20-24, 2015
Telluride



Telluride Science Research Center

Organizers: Ferdinand Evers, Michael Thoss, and Latha Venkataraman

TSRC Hosts: Mark Kozak 970-708-4426

Location: Telluride Elementary School, 477 West Columbia Ave, Telluride,
CO 81435

	Monday	Tuesday	Wednesday	Thursday	Friday
8:00 am	Breakfast	Breakfast	Breakfast	Breakfast	Breakfast
8:30 am					
9:00 am	J. van Ruitenbeek 8:40-9:40	H. van der Zant 8:30-9:10	free	H. Wang 8:30-9:10	Group hike
9:30 am		T. Frederiksen 9:10-9:50		G. Cohen 9:10-9:50	
10:00 am	A. Nitzan 9:40-10:20	M. Thoss 9:50-10:30		M. Galperin 9:50-10:30	
10:30 am	Coffee Break	Coffee Break		Coffee Break	
11:00 am	C. Nijhuis 10:50-11:30	L. Venkataraman 11:00-11:40		E. Rabani 11:00-11:40	
11:30 am	M. Reuter 11:30-12:10	U. Peskin 11:40-12:20	F. Evers 11:40-12:20		
12:00 am					
12:30 am					
1:00 pm					
1:30 pm					
2:00 pm			E. Scheer 13:30-14:10		
2:30 pm	R. Naaman 14:00-14:40	N. Agrait 14:00-14:40	O. Monti 14:10-14:50	F. Giessibl 14:00-14:40	
3:00 pm	M. Ternes 14:40-15:20	C. Stafford 14:40-15:20	P. Zolotavin 14:50-15:10	G. Solomon 14:40-15:20	
3:30 pm	Coffee Break	Coffee Break	Coffee Break	Coffee Break	
4:00 pm	O. Tal 15:50-16:30	P. Reddy 15:50-16:30	Y. Selzer 15:40-16:10	J. Neaton 15:50-16:50	
4:30 pm					
5:00 pm	R. Korytar 16:30-16:50	Y. Dubi 16:30-17:10	G. Chen 16:10-16:50		
5:30 pm					
6:00 pm					
6:30 pm		TSRC Town Talk 18:00-19:00	TSRC Picnic BBQ 18:00-21:00		
7:00 pm		Telluride Confer- ence Center in Mountain Village	Telluride Elemen- tary School		
7:30 pm					
8:00 pm					

Monday

8:30–8:40 Opening

Morning Session

Chair: Latha Venkataraman

8:40–9:40 Jan van Ruitenbeek Molecular junctions: what we know, and what we do not know (+ Overview)

9:40–10:20 Abraham Nitzan Current transfer, circular currents, magnetic field effects and spin selectivity in molecular conduction

10:20–10:50 Coffee Break

10:50–11:30 Christian Nijhuis Molecular "Super" diodes

11:30–12:10 Matthew Reuter Quantitative interpretations of conductance histograms in molecular electron transport

Afternoon Session

Chair: Thomas Frederiksen

14:00–14:40 Ron Naaman Spin selective transport through nanoscale molecular systems

14:40–15:20 Marcus Ternes Revealing higher order scattering effects and induced correlations in atom and molecular spin systems by STM

15:20–15:50 Coffee Break

15:50–16:30 Oren Tal Spin filtering and enhanced magnetoresistance in atomic and molecular junctions

16:30–16:50 Richard Korytar Quantum size effect and Kondo side-peaks in electronic transport through organic molecules

Tuesday

Morning Session

Chair: Pramod Reddy

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| 8:30–9:10 | Herre van der Zant | OPE-3: a fruitfly molecule for studying transport mechanisms |
| 9:10–9:50 | Thomas Frederiksen | DFT-based methods for electron-phonon couplings and quantum transport - recent developments and applications |
| 9:50–10:30 | Michael Thoss | Charge transport in molecular junctions: Vibrational effects, density matrix theory, and graphene electrodes |

10:30–11:00

Coffee Break

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| 11:00–11:40 | Latha Venkataraman | Measurements of voltage-induced single-molecule junction rupture in silicon-based molecular wires |
| 11:40–12:20 | Uri Peskin | Charge transport induced dissociation of double dots: The role of electronic interactions and quantum interference |

Afternoon Session

Chair: Oren Tal

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|-------------|------------------|---|
| 14:00–14:40 | Nicolas Agrait | Thermopower control in molecular junctions |
| 14:40–15:20 | Charles Stafford | Local thermodynamics of a nonequilibrium quantum system |

15:20–15:50

Coffee Break

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| 15:50–16:30 | Pramod Reddy | Radiative heat transfer at the nanoscale |
| 16:30–17:10 | Yonathan Dubi | Pushing (and pulling) the limits of thermoelectricity in molecular junctions |

Wednesday

Afternoon Session

Chair: Abraham Nitzan

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|-------------|-----------------|--|
| 13:30–14:10 | Elke Scheer | Atomic and molecular switches |
| 14:10–14:50 | Oliver Monti | New avenues to reveal the influence of electrostatics on transport |
| 14:50–15:10 | Pavlo Zolotavin | Voltage tuning of vibrational mode energies and optically induced changes to the tunneling properties of molecular junctions |

15:10–15:40

Coffee Break

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| 15:40–16:10 | Yoram Selzer | Plasmonic effects in molecular junctions |
| 16:10–16:50 | Guanhua Chen | Time-dependent processes in molecular dynamics |

Thursday

Morning Session

Chair: Charles Stafford

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| 8:30–9:10 | Haobin Wang | Transient dynamics in the time-dependent quantum transport |
| 9:10–9:50 | Guy Cohen | Taming the dynamical sign problem: the Inchworm algorithm |
| 9:50–10:30 | Michael Galperin | Energy transport and heating in an open quantum nanoscale device |

10:30–11:00

Coffee Break

11:00–11:40 Eran Rabani tba

11:40–12:20 Ferdinand Evers Many-body perturbation theory for single molecules: status, issues, prospects

Afternoon Session

Chair: Elke Scheer

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|-------------|----------------|---|
| 14:00–14:40 | Franz Giessibl | Revealing electron clouds, spins and bonds with the force microscope |
| 14:40–15:20 | Gemma Solomon | Calculation without computation: predicting molecular conductance from chemical structure alone |

15:20–15:50

Coffee Break

15:50–16:50 Jeffrey Neaton Consequences of collective solvent behavior in molecular junctions (+ Summary)

16:50–16:55

Closure