



Quantum Transport in Nanoscale Molecular Systems

July 29 - August 2, 2019
Telluride



Telluride Science Research Center

Organizers: Ferdinand Evers, Michael Thoss, and Latha Venkataraman

TSRC Hosts: Mark Kozak 970-708-4426

Location: Telluride Intermediate School, 725 W Colorado Ave, Telluride,
CO 81435

	Monday	Tuesday	Wednesday	Thursday	Friday
8:00 am	Breakfast	Breakfast	Breakfast	Breakfast	Breakfast
8:30 am	Opening	P. Jelinek 8:30-9:10	Hiking/discussions	G. Solomon 8:30-9:10	Hiking/discussions
9:00 am	K. Franke 8:40-9:40	J. Pascual 9:10-9:50		T. Frederiksen 9:10-9:50	
9:30 am				Coffee Break	
10:00 am	W. Wulfhekel 9:40-10:20	S. Gunasekaran 9:50-10:10		O. Tal 10:20-11:00	
10:30 am	Coffee Break	Coffee Break		T. Novotny 11:00-11:40	
11:00 am	A. Nitzan 10:50-11:30	S. Refaelly- Abramson 10:40-11:20	Lunch Break		
11:30 am	M. Thoss 11:30-12:10	A. Donarini 11:20-12:00			
12:00 am		Lunch Break			
12:30 am	Lunch Break				
1:00 pm					
1:30 pm			M. Brandbyge 13:30-14:10		
2:00 pm	U. Peskin 14:00-14:40	J. Thijssen 14:00-14:40	Coffee Break	C. Stafford 14:00-14:40	
2:30 pm	D. Perez 14:40-15:00	P. Hedegard 14:40-15:20		F. Evers 14:40-15:40	
3:00 pm	Coffee Break	Coffee Break			
3:30 pm	F. Fischer 15:30-16:10	M. Hybertsen 15:50-16:30	G. Schull 15:20-16:00		
4:00 pm			I. Franco 16:00-16:40		
4:30 pm					
5:00 pm					
5:30 pm					
6:00 pm			TSRC Picnic BBQ 18:00-20:00		
6:30 pm		TSRC Town Talk 18:30-19:30	Telluride Intermediate School		
7:00 pm		Telluride Conference Center in Mountain Village			
7:30 pm					
8:00 pm					

Monday

8:30–8:40		Opening

Morning Session		Chair: Gemma Solomon
8:40–9:40	Katharina Franke	Single-layer MoS ₂ on Au(111) as decoupling layer for molecules: Molecular vibrations and radicals (+ Overview)
9:40–10:20	Wulf Wulfhekel	Functional molecular tripods

10:20–10:50		Coffee Break

10:50–11:30	Abraham Nitzan	Wiedemann-Franz law for molecular hopping transport
11:30–12:10	Michael Thoss	Hierarchical quantum master equation approach to charge transport in molecular junctions

Afternoon Session		Chair: Elke Scheer
14:00–14:40	Uri Peskin	Mechanically stable molecular junctions during resonant transport ?
14:40–15:00	Daniel Hernangomez Perez	Mechanically-tunable quantum interference in Ferrocene-based single-molecule junctions

15:00–15:30		Coffee Break

15:30–16:10	Felix Fischer	Forging symmetry protected topological states into metallic graphene nanoribbons

Tuesday

Morning Session

Chair: Wulf Wulfhekel

8:30–9:10 Pavel Jelinek

1D organometallic chains: on-surface synthesis and transport

9:10–9:50 Jose Ignacio Pascual

Spin detection and manipulation in graphene open shell nanostructures

9:50–10:10 Suman Gunasekaran

Tight-binding analysis of helical orbitals and ring currents in sp-carbon chains

10:10–10:40

Coffee Break

10:40–11:20 Sivan Refaelly-Abramson

First principles approach to the conductance of covalently bound molecular junctions

11:20–12:00 Andrea Donarini

Dark states in a carbon nanotube quantum dot

Afternoon Session

Chair: Charles Stafford

14:00–14:40 Jos Thijssen

Symmetry, spin selectivity and spin-orbit interaction

14:40–15:20 Per Hedegård

Theory of chiral induced spin selectivity

15:20–15:50

Coffee Break

15:50–16:30 Mark Hybertsen

Exploring structure-conductance relations with model Hamiltonians

Wednesday

Afternoon Session

Chair: Jose Ignacio Pascual

13:30–14:10 Mads Brandbyge Current-induced forces and multi-scale calculations of transport in molecular structures

14:10–14:50 Elke Scheer Atomic and molecular contacts under strong bias:
Phonon-mediated switching and limitations of the single-level model

14:50–15:20 Coffee Break

15:20–16:00 Guillaume Schull From sub-molecular fluorescence microscopy to fluorescent molecular junctions

16:00–16:40 Ignacio Franco Frontiers in the atomistic modeling of single-molecule force-conductance spectroscopies

Thursday

Morning Session		Chair: Mads Brandbyge
8:30–9:10	Gemma Solomon	Helical orbitals and circular currents in cumulenes
9:10–9:50	Thomas Frederiksen	Electron transport in multi-terminal devices

9:50–10:20	Coffee Break	

10:20–11:00	Oren Tal	The effect of magnetic field on the properties of chemical bonds in atomic and molecular junctions
11:00–11:40	Tomas Novotny	Three short Kondo pieces (for the experiment, NRG, and analytic considerations)
Afternoon Session		Chair: Abraham Nitzan
14:00–14:40	Charles Stafford	Topological effects in quantum thermodynamics
14:40–15:40	Ferdinand Evers	Developments in molecular Electronics - a theorists perspective (+ Summary)
15:40–15:50	Closure	