QuIET

Quantum Interference Enhanced Thermoelectricity

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Abstract

Our vision is to demonstrate that room-temperature quantum interference effects, measured recently in single molecules, can be exploited in massively-parallel arrays of molecules and used to design ultra-thin-film thermoelectric devices with unprecedented ability to convert waste heat to electricity using the Seebeck effect and to cool at the nanoscale via the Peltier effect.

Although the dream of high-performance thermoelectric devices has been discussed for many years, evidence of the room-temperature quantum interference effects needed to realise this dream was achieved experimentally only recently. Building on these indirect demonstrations of quantum interference in single molecules using non-scalable setups, we anticipate that the next breakthrough will be the implementation of QI functionality these in technologically relevant platforms.

Abstract (continued)

We shall design molecules with built-in quantum interference functionality, which can be used to engineer the properties of ultra-thin molecular films. Molecules will be designed with robust anchors to metallic and carbon-based nano-gap electrodes, which enhance electron transport and eliminate unwanted phonons. This contacting strategy is scalable from a single junction, with the potential to be replicated billions of times on a single substrate. The ability to exploit quantum interference at room temperature will enable new thermoelectric materials and devices with the ability to scavenge energy with unprecedented efficiency.

QuIET is a highly interdisciplinary project that brings together internationally leading scientists from four different countries with proven expertise on synthesis, transport measurements and theoretical modelling.

Project Partners

Coordinator: Prof. Nicolás Agrait

Prof. Colin J Lambert

Prof. Herre van der Zant

Prof. Martin R. Bryce

Dr. Bernd Gotsmann

Prof. Marcel Mayor

Dr. Michel Calame

Research Approach

We will design, synthesise and characterise molecules and molecular films with QI-enhanced thermoelectric functionality and explore the feasibility of building efficient thermoelectric devices.

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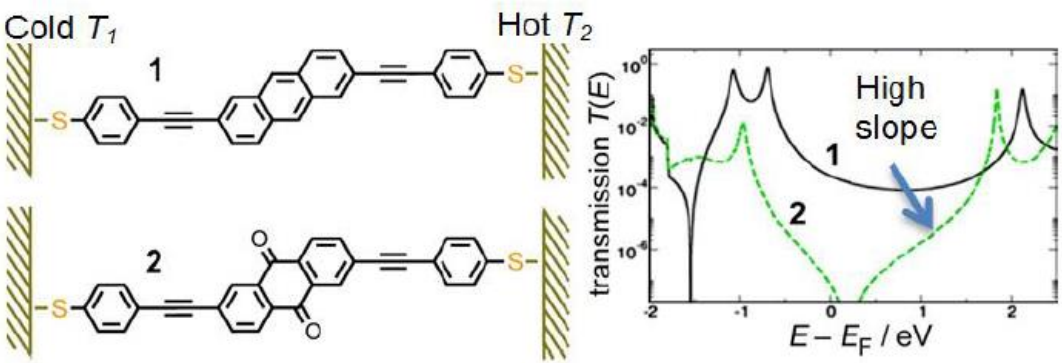

Single molecule junctions show Quantum Interference effects leading to a high slope in the transmission function, and consequently high Seebeck coefficient

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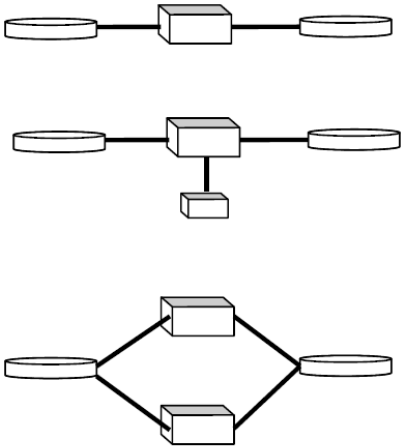
Quantum Interference in molecular junctions



Breit-Wigner

Fano

Mach-Zehnder

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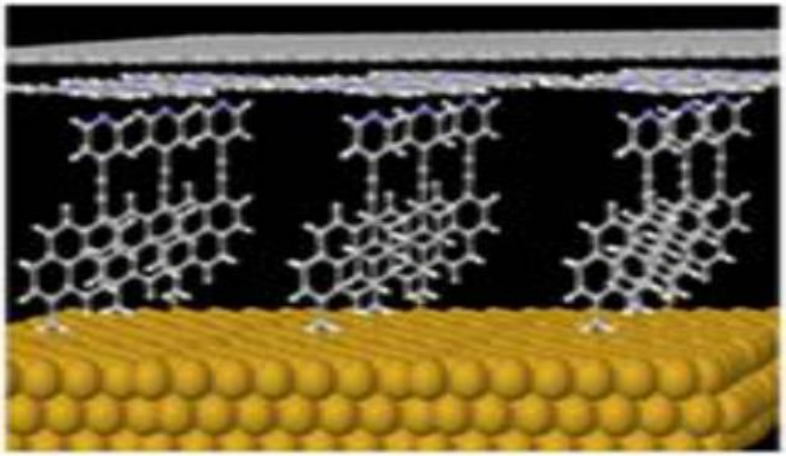
Parallel array of molecules



Methodology

1. Synthesis of prototype molecules that are predicted to present QI effects leading to high thermopower.

2. Fast screening of single-molecule junctions built with the molecules synthesised in step 1 using scanning probe techniques to identify molecules that show high thermopower.

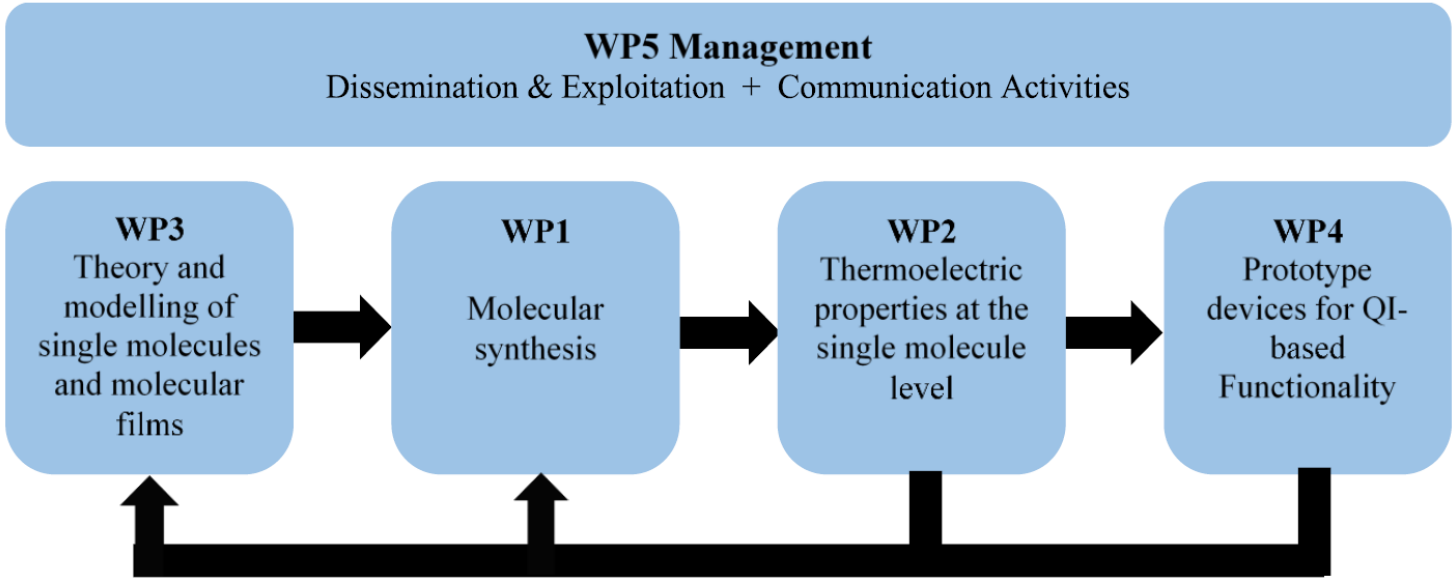
3. Detailed characterisation of junctions of molecules selected in the previous step using various techniques to gain insight on the interplay between electrical transport, electronic resonances and thermopower.

4. For full *ZT* characterisation of the single-molecule junctions, we will measure thermal conductance using novel MEMs-based sensors and hot-wire techniques.

5. Exploration of how the thermoelectric properties behave in relevant device geometries using self-assembled monolayers.

6. Exploration of device configurations optimized with respect to performance and manufacturability taking into account the requirements of diverse applications

Implementation



Implementation (Gantt chart)

		SEMESTER						
		1	2	3	4	5	6	7
WP1	Task 1.1	D1.1	M2					
	Task 1.2		D1.2					
	Task 1.3				D1.3		D1.5	
	Task 1.4				M5 D1.4		M10 D1.5	D1.6
WP2	Task 2.1		M2 D2.1					
	Task 2.2		M3	D2.2				
	Task 2.3			M4				D2.4
	Task 2.4				M9	D2.3		
WP3	Task 3.1		M1 D3.1	D3.2	M6		M11	M13
	Task 3.2							
	Task 3.3							
	Task 3.4				D3.3	D3.4		M12 D3.5
WP4	Task 4.1				M5			
	Task 4.2		M3 D4.1			D4.4		D4.5
	Task 4.3				M7 D4.2			
	Task 4.4				M8 D4.3			D4.6
WP5	Task 5.1			D5.5		D5.7		D5.13
	Task 5.2		D5.4		D5.6			D5.12
	Task 5.3	D5.1 D5.2 D5.3				D5.8	D5.9	D5.10 D5.11

WP 1 Molecular synthesis

Objectives: Synthesis of molecules with enhanced thermoelectrical properties.

Task 1.1. Molecules for single-point contacts to metals. (UDUR, UBAS)

Task 1.2 Large-area, π-stacking contacts and multiple-interaction contacts. (UBAS, UDUR)

Task 1.3. Polycyclic wires. (UBAS)

Task 1.4. Cross-linked structures in SAMs. (UDUR)

WP 2 Thermoelectric properties at the single molecule level

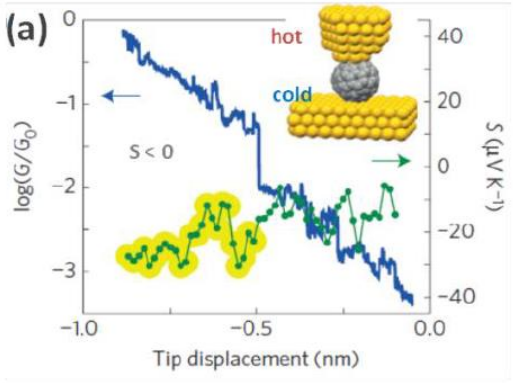
Objectives. We will screen molecules for optimal thermoelectric properties and extensively characterize selected molecules to achieve controllable thermoelectric properties in molecular junctions (MJs).

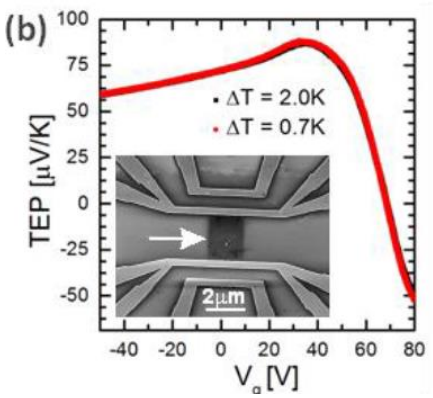
Task 2.1. Fast screening. (UAM, IBM)

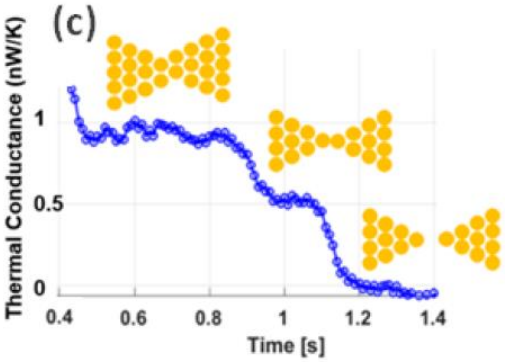
Task 2.2. Conductance and electronic transmission. (EMPA, TUD, UAM, IBM)

Task 2.3. Thermopower characterization and control. (EMPA, TUD, UAM, IBM)

Task 2.4. Thermal conductance in molecular junctions. (IBM, UAM)







WP 3 Theory and modelling of single molecules and molecular films (ULAN)

Objectives. Design, simulation and modelling of whole devices, including the environment and intermolecular interactions. Modelling of electron and phonon contributions to thermoelectricity. New release of the multi-scale simulation capability 'Gollum,' which interfaces quantum mechanical simulations for electrical and thermal transport with classical molecular dynamics simulations of the environment.

Task 3.1. New release of a multi-scale simulation tool "Gollum" for molecular-scale electronics, thermoelectrics and phonon transport in realistic environments.

Task 3.2 Investigations of the stability of candidate anchor units.

Task 3.3. Controlling QI in molecular wires.

Task 3.4. Understanding and controlling the effect of a surrounding medium and intermolecular interactions.

WP 4 Prototype devices for QI-based Functionality

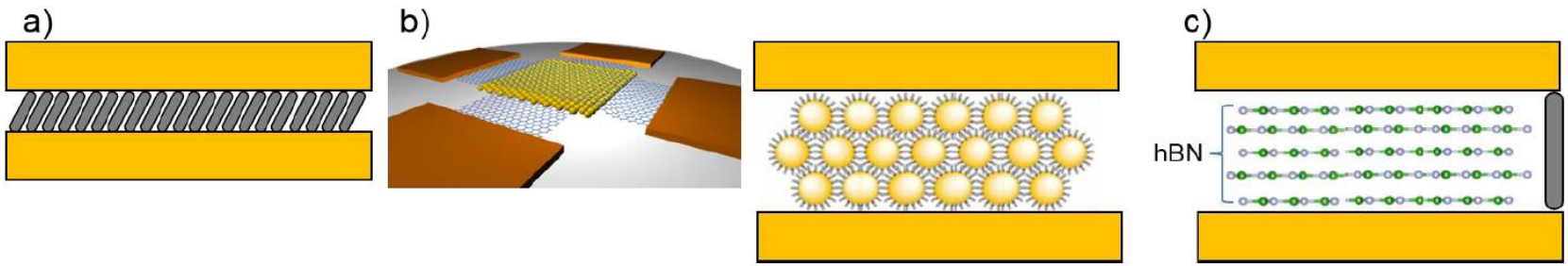
Objectives. To explore integration avenues of materials exploiting QI mechanisms in future devices and to perform a quantitative and complete thermoelectric characterization of different candidate architectures.

Task 4.1 Thermopower and electrical conductance measurements. (IBM, UAM)

Task 4.2 Thermal conductance measurements. (IBM, UAM)

Task 4.3 Nanoparticle arrays. (EMPA, UAM)

Task 4.4 Hybrid vertical junctions. (TUD, IBM, EMPA)



WP 5 Management

Objectives This WP will establish the management structure and procedures which regulate the activities of the network and implement a series of actions aimed at maximising the impact of QuIET through dissemination and exploitation.

Task 5.1. Management.

Task 5.2. Dissemination and exploitation.
Plan dissemination and exploitaition of QuIET's results

Task 5.3. Communication activities.
Outreach activities and establishment of a public website

Summary of project effort in person-months

	WP1	WP2	WP3	WP4	WP5	Total Person/Months per Participant
1 - UAM	1	46	1	32	22	102
2 - ULAN	1	1	31	1	2	36
3 - TUD	1	23	1	26	2	53
4 - UDUR	41	1	1	1	2	46
5 - IBM	1	16	1	16	2	36
6 - UBAS	50	1	1	1	2	55
7 - EMPA	1	26	1	24	2	54
Total Person/Months	96	114	37	101	34	382

Relevance of expertise in the consortium: Complementary expertise

Recognized experts in molecular electronics + leading industrial research laboratories
1,300 papers, 45,000 citations, 90 patents

UDUR and **UBAS**: synthesis of molecules with enhanced thermoelectric properties and anchor groups adequate to the different electrodes.

ULAN: modelling and theoretical simulations, guide the design and synthesis of molecules with enhanced thermoelectric properties

Characterisation molecular junctions and self-assembled monolayers using state-of-the-art tools: scanning probes (**UAM** and **IBM**), mechanically controlled break-junctions, electromigrated metal junctions and electroburnt graphene junctions (**EMPA** and **TUD**).

UAM and **IBM**: Measurement of thermal conductance at single molecule level.

TUD: fabrication and measurement of the hybrid vertical junctions, using their extensive infrastructure of the Nanofacility of the Kavli Institute of Nanoscience with its state-of-the-art cleanroom.

EMPA: hybrid co-planar and vertical nanoparticle arrays using graphene electrodes.

Some advice…

- Clear objectives: a focused proposal
- Good partners
- Experience in previous EC Projects as partner