



Institute for Materials Science, Chair of Materials Science and Nanotechnology

# **Quantum Transport and Thermoelectric Efficiency in Low-Dimensional Systems**

### **Kick off TAC**

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## **Motivation**

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The evolution of electronic systems is heading a heat management challenge.







Thermal fluctuations play an important role in biological systems.



# **Previous work: Master thesis**

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### Atomistic study of heat flow in molecular heterojunctions

To control the heat flow at the nanoscale



#### 1. Phonon filter

Phonon filter from an electronic analog.

Manuscript submitted. Medrano S, Rodriguez A, Gutierrez R, Ugalde J, Mujica V, Cuniberti G. Selective Transmission of Phonons in molecular Junctions with Nanoscopic Therml Baths, Journal of Phys. Chem.

#### 2. Nanoscale phononic analog of Ranque-Hilsch vortex tube $T_{A} < T_{B}$ А Generate $\geq$ а temperature gradient employing a single heat source. Manuscript in work. Medrano S, Rodriguez A, Gutierrez R, Ugalde J, Mujica V, Cuniberti G. A nanoscale analog of the Ranque-Hilsch Vortex Tube.

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### **Phonon filter**

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## **Ranque-Hilsch Vortex Tube**

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## Actual topics: PhD thesis (Months 1-8)

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#### 1. Nanoscale phononic analog of Ranque-Hilsch vortex tube on Si surface.



- $\triangleright$
- Study the influence of a Si in the temperature bias.

#### 2. Development of thermoelectric devices based on dendrimers

Thermoelectric properties of dendrimers connected with graphene nanorribons by covalent bonds, pi-stack interaction and both interactions.



#### 3. Improvement of the figure of merit in thermoelectric devices by CNT peapods.



Study the effect of the fullerenes in the thermoelectric transport of the CNT.



# **Ranque-Hilsch Vortex Tube**

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Actual tasks:

- Determine how the Si surface influences the temperature bias of the suspended system by computing the density of states.

- Complete the paper.





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- Actual tasks:
- Compute thermal transport of dendrimers A and B displaced between two graphene nanoribbons with covalent bonds and as pi-stacked system.
- ➢ Future tasks:
- Compute electronic transport in these systems
- Test dendrimers with higher number of generations

Li, Q. *et al. A Strategy to Supress Phonon Transport in molecular Junctions Using pi-Stacked Systems*. J. Phys. Chem. **121**, 7175–7182 (2017). Borjesson, K. *et al.* Conjugated anthracene dendrimers with monomer-like fluorescen. *RSC Adv.* **4**, 19846–19850 (2014).





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- Actual tasks:
- Reproduce the deformation of the CNT with DFTB method.
- ➢ Future tasks:
- Compute thermoelectronic transport and anharmonic contribution in CNT peapods.
- Test effect on different CNT (8,8; 9,9)
- Test different fullerene cages and hybrid systems
- Change material of NT