



From Materials to Devices

The importance of physics in material science & technology for sustainable energy applications

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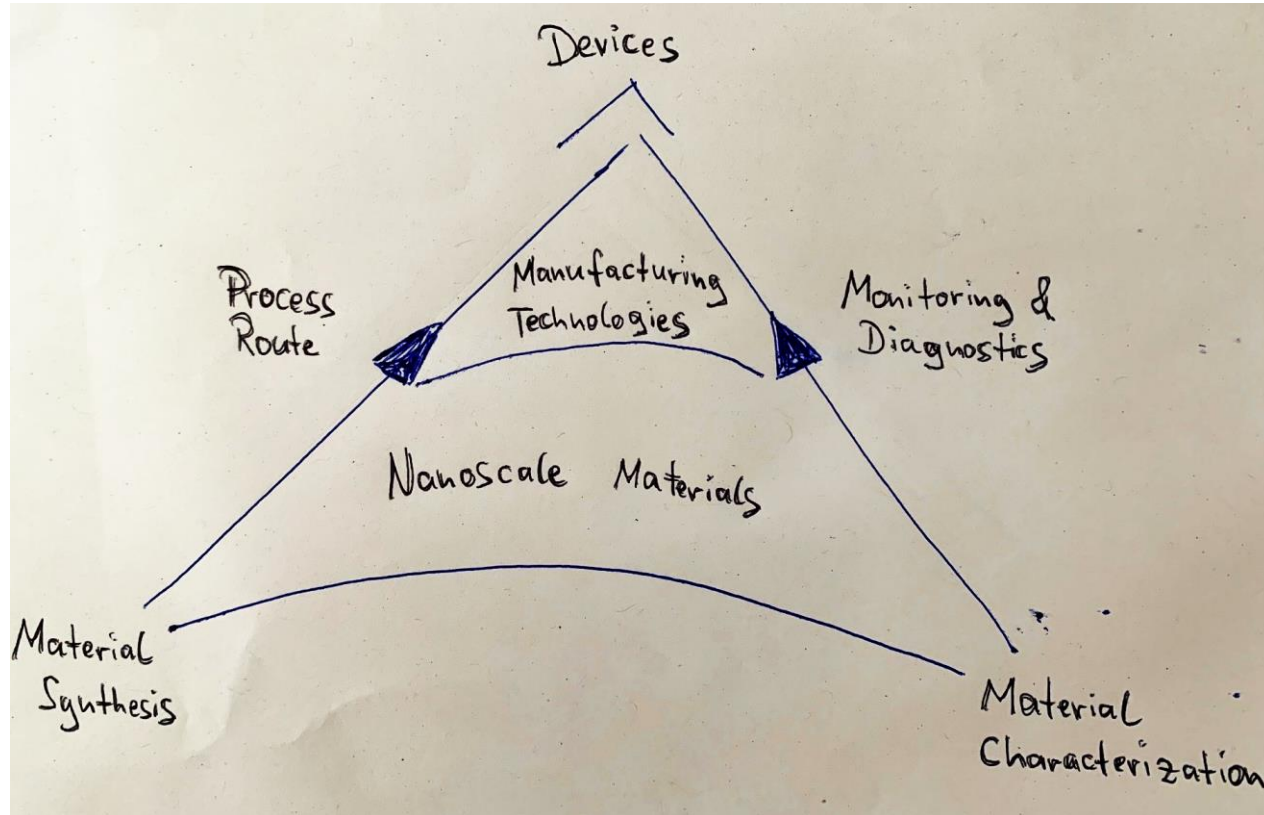
SPS Annual meeting 2024-09-13, ETHZ

Outline



- Introduction:
 - Concept «Materials to Devices»
 - Physics in Energy-related Materials Science at Empa
- Example 1: High Efficiency CIGS solar cells
- Example 2: Solid state thin film batteries
- Example 3: Quantum heat engines as thermoelectric generators
- Summary

Introduction: From Materials to Devices...



Energy supply, conversion and storage

- Photovoltaics
- Batteries
- Power to X
- Seasonal thermal storage

System integration

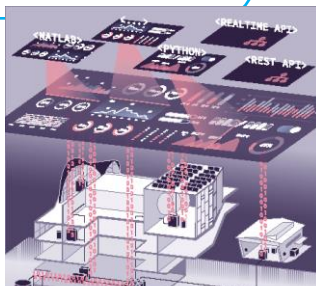
- Supply & demand balancing
- Sector coupling
- Resilient energy system
- Demonstrators & case studies

Energy Demand

- Energy-efficient materials & processes
- Circular construction & retrofitting
- Building monitoring & operation
- E- and H₂-mobility, synthetic fuels



NEST



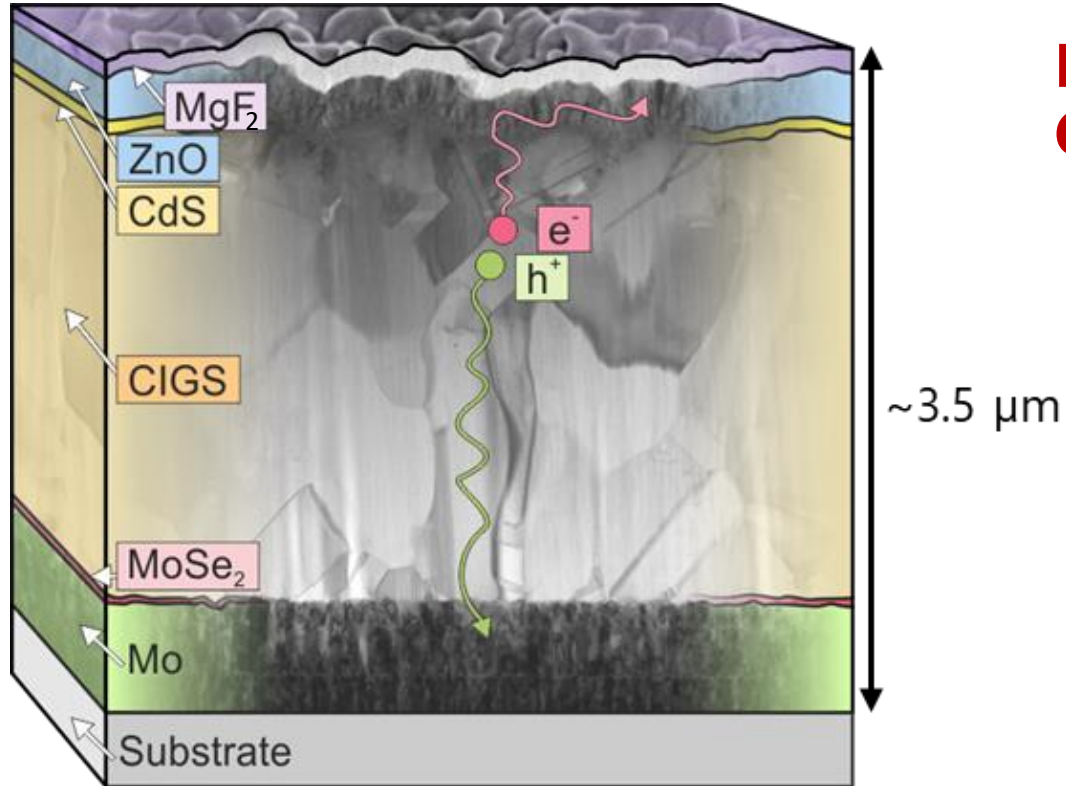
Energy Hub



move



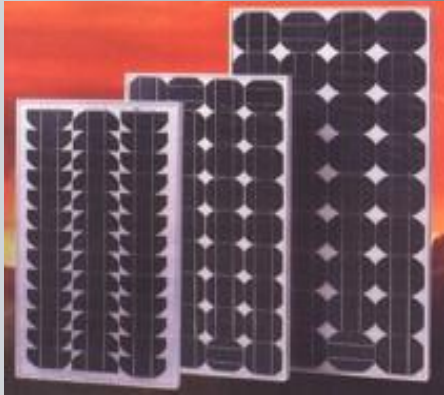
High Efficiency CIGS $\text{Cu}(\text{In},\text{Ga})\text{Se}_2$ solar cells



Generations of solar cells



1st Generation: Silicon wafer-based



- Wafer thickness: 200 μ m
- Rigid
- Heavy

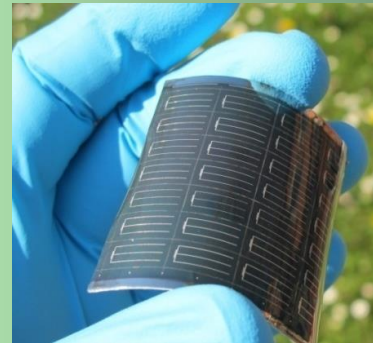
- 55 years old
(95% market share)

2nd Generation: Thin-films: CdTe, CIGS,...



Rigid substrate

- Absorber thickness:
<3 μ m but still heavy
- Large area deposition
- Monolithic integration

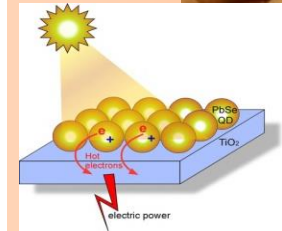
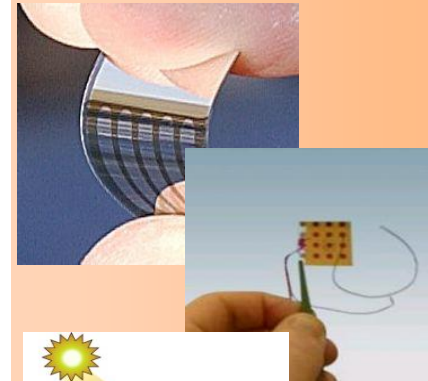


Flexible Light-weight

R-2-R

- 20 years old (5% market share)

3rd Generation: new concepts such as Bifacial, tandem,



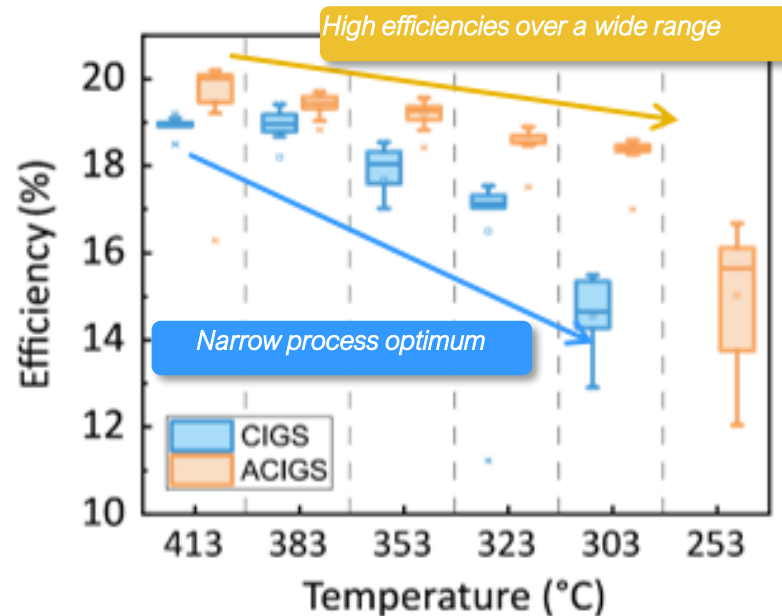
High-EFFICIENCY flexible solar cells @ Empa



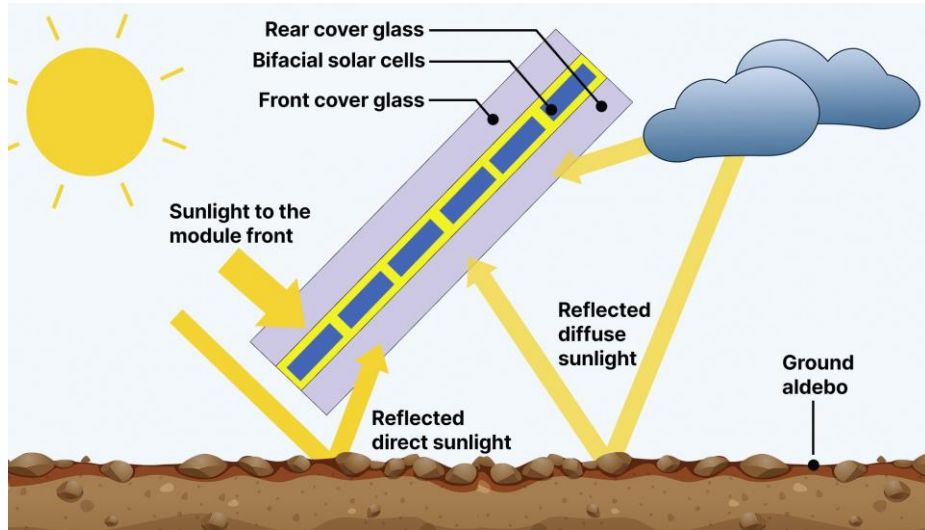
Approach: absorber alloying

- Tiny amounts of silver in CIGS
- Improved PV performance:
Power conversion efficiency >22%
- Improved Process tolerance
- Low temperature process enabling polymer or other delicate substrates

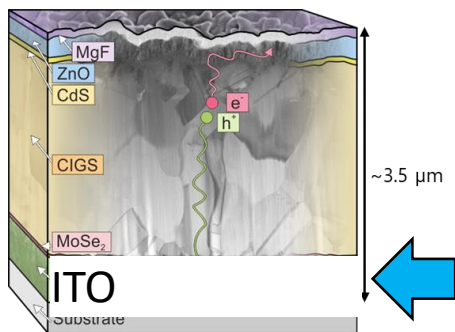
Can we bring up efficiency even further?



Idea: Bifacial CIGS solar cells



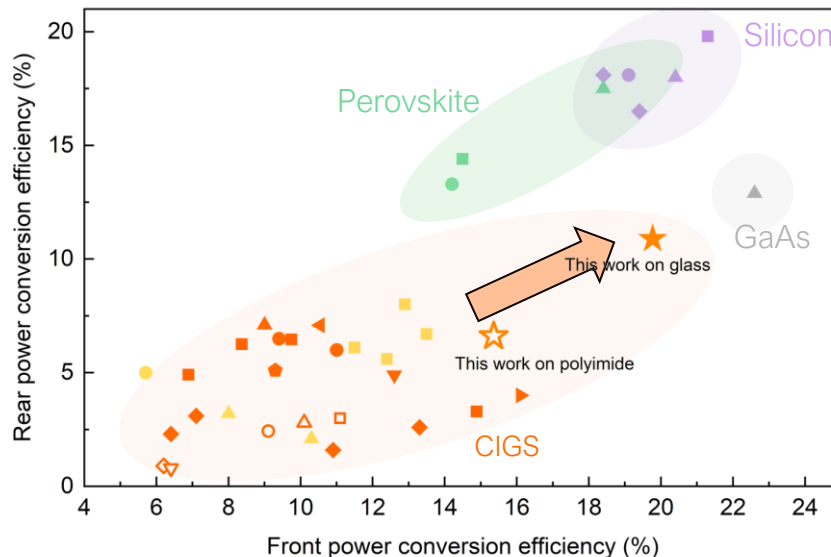
What about bifacial CIGS ?



Our approach

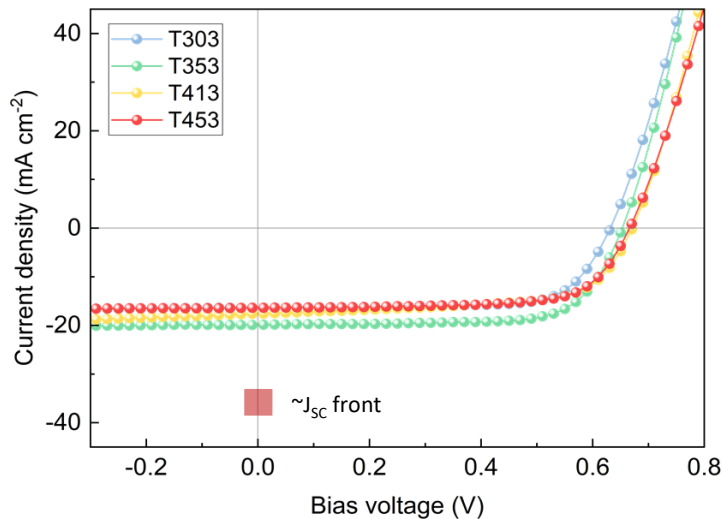
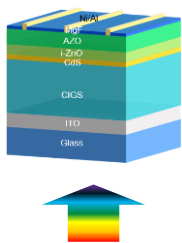
- Replace metal Mo with transparent ITO (possible due to low process temperature of Ag alloyed material!)

Can we bring up efficiency even further?

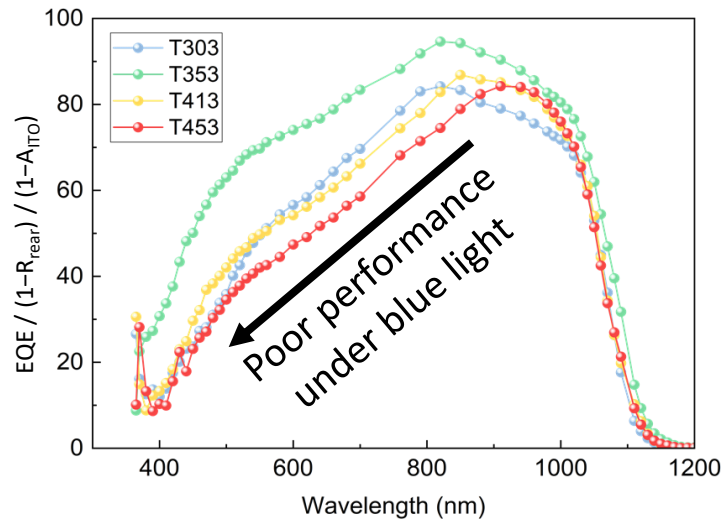


- **Breakthrough: devices work well!**
- Romain Carron – Yaroslav Romanyuk

Physical limits: low photocurrent under rear illumination

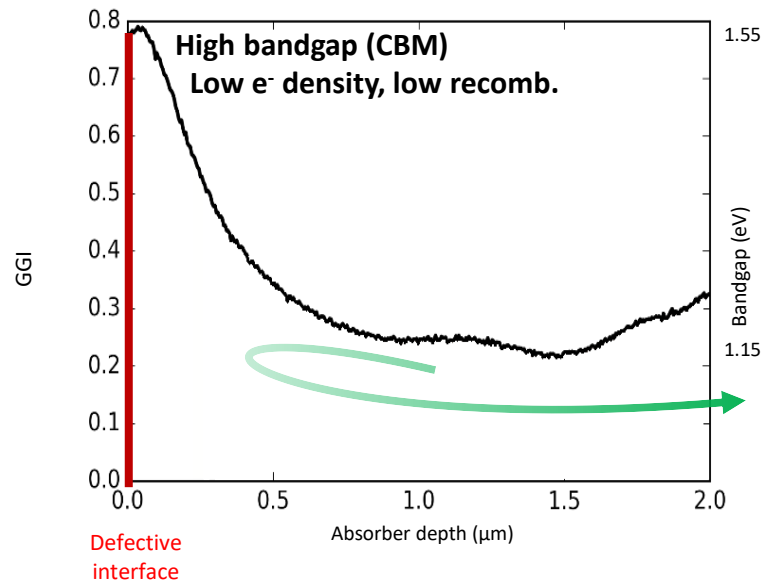
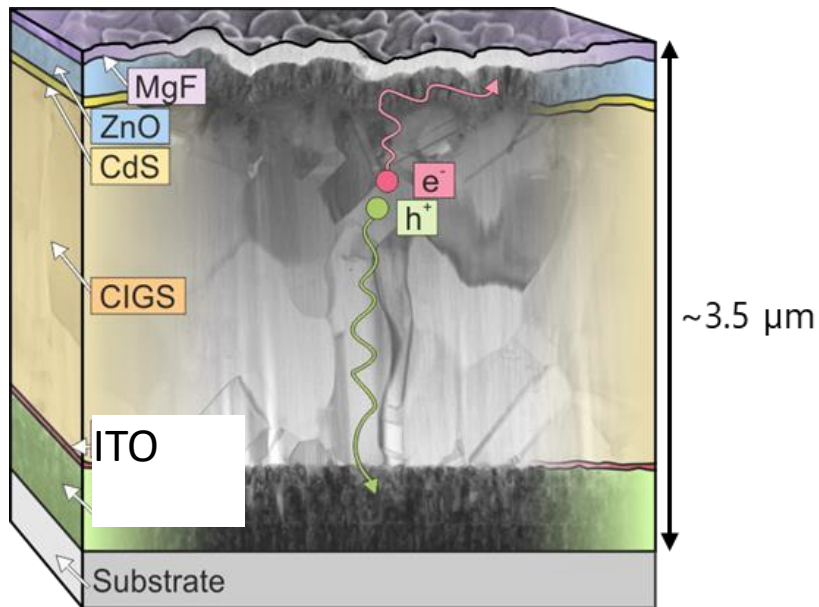


Rear illumination: missing about half photocurrent



External quantum efficiency corrected for absorption and reflection

Bandgap gradient

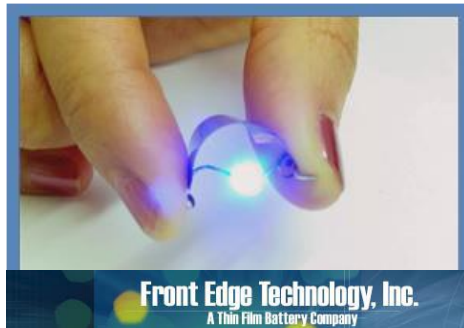
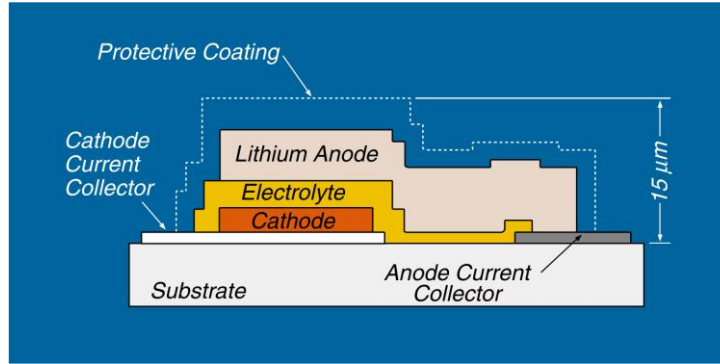


Issue: big bandgap at rear interface

- Low electron density, low recomb.
- Bad efficiency to create backside e-h pairs

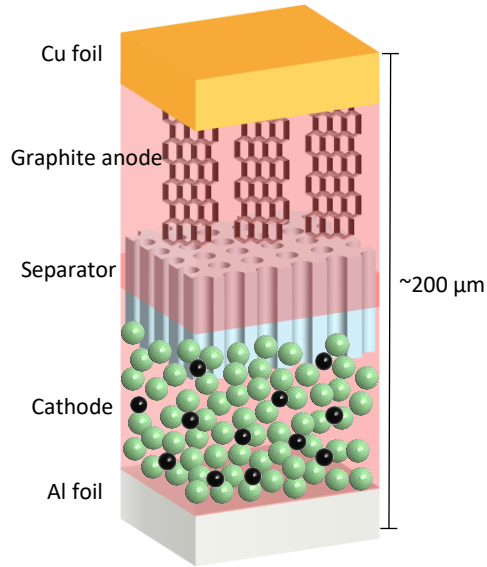
Outlook: absorber without gradient/
charge selective contacts

Thin-film batteries (TFB)

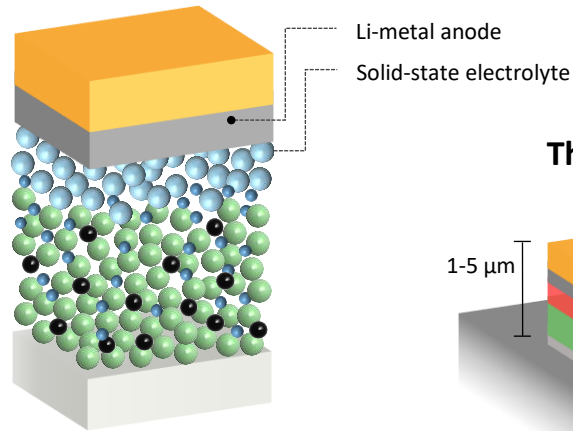


TFB is a miniature solid-state battery

Li-ion battery



Solid state battery (SSB)



Thin-film battery (TFB)

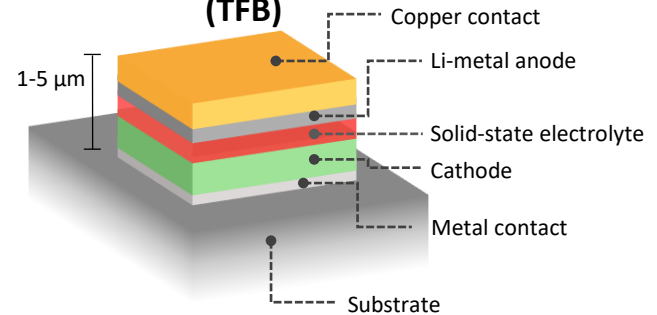
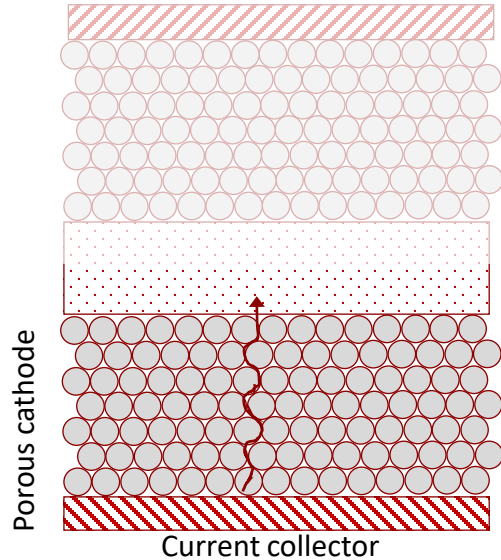


Image courtesy: Xinyao Li

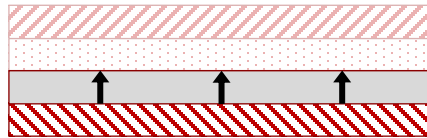
Ion diffusion path determines charging rate

Li-ion battery



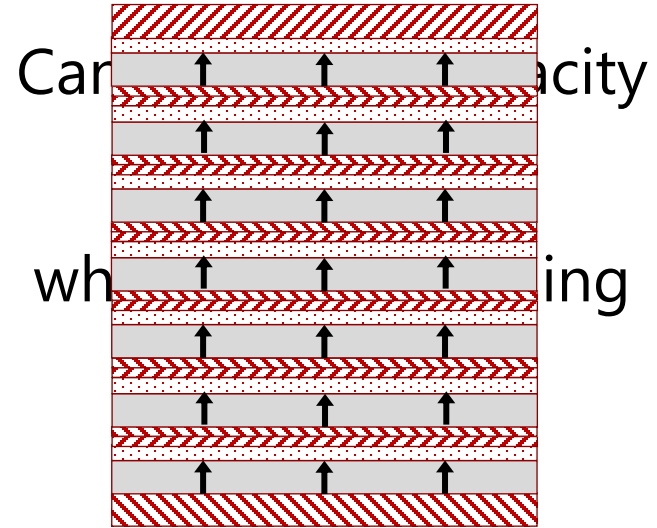
high energy
low rate

Thin-film battery



very low energy
high rate

Monolithic multi-cell
thin-film battery!?



high energy
high rate

Thin-film battery fabrication line at Empa

ALD



Magnetron sputtering

Wet glovebox

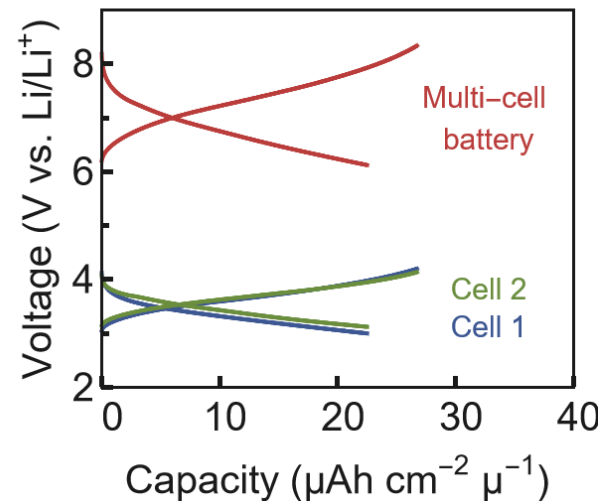
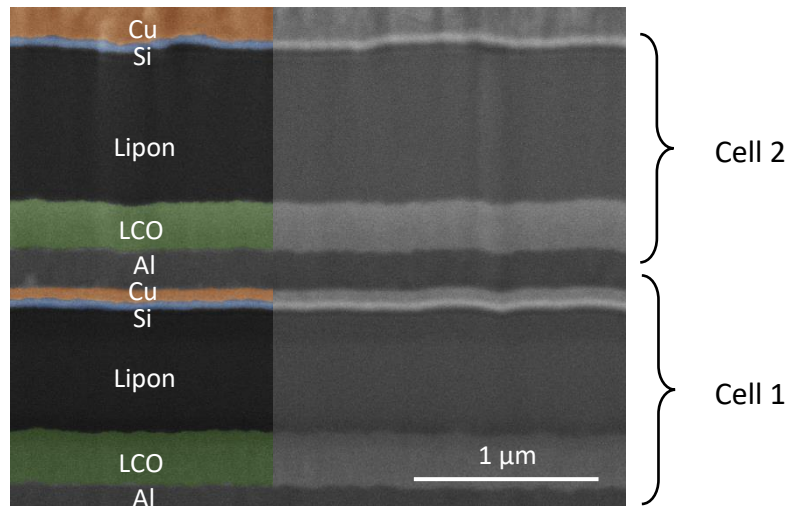
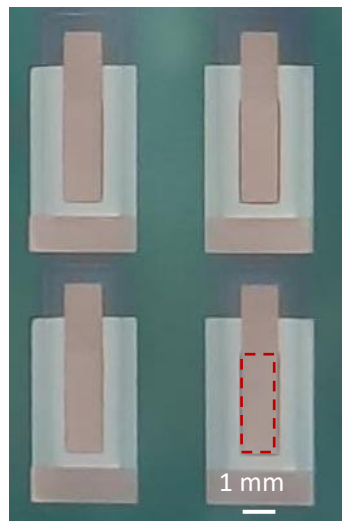
Dry glovebox

Thermal evaporator

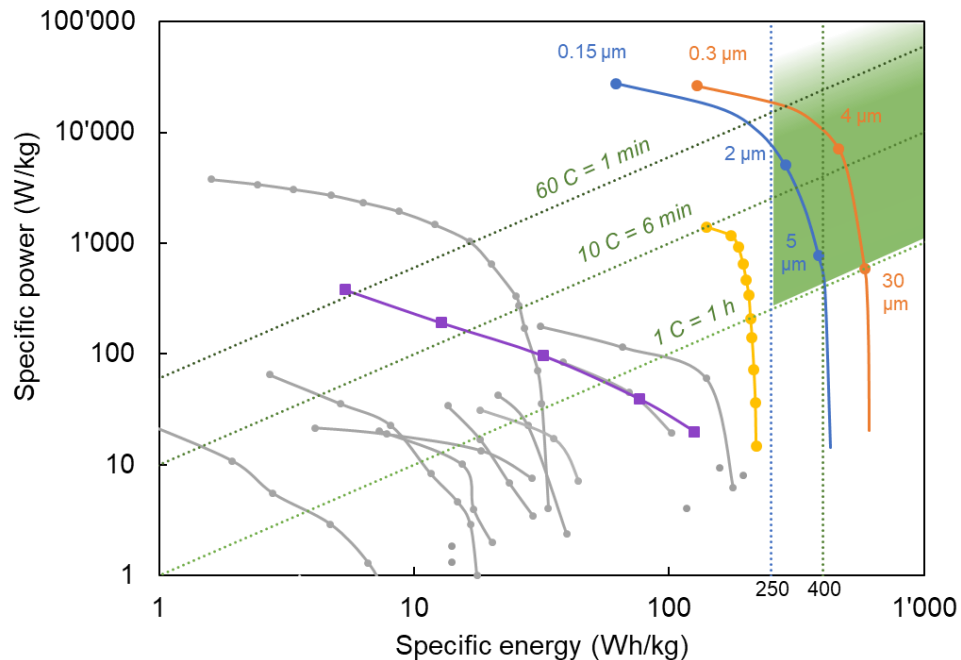


FLA

Experimental proof of concept: the first tandem stacked thin-film battery



Benchmarking with solid-state batteries



— Solid-State Batteries (SoA)*

* S. Randau *et al.* Nat Energy 5, 259–270 (2020)

— This work (experimental)

— LG 18650 HG2L 3000 mAh

— This work (NMC811, modeled)

— This work (LCO, modeled)

Enabling high power and high
Energy in one device!

Empa spin-off BTRY AG

"A sustainable, reliable solid-state Li-ion battery that can be charged in one minute."

Li-ion battery



BTRY



Supercapacitor



M. Futscher & A. Aribia

spin-off | Empa

High-Tech Gründerfonds

IBAT

WISSENSCHAFT.
BEWEGEN
GEBERT RUF-STIFTUNG

BÜROZÜRI
by Zürcher Kantonalbank

Spin-off | ETH zürich

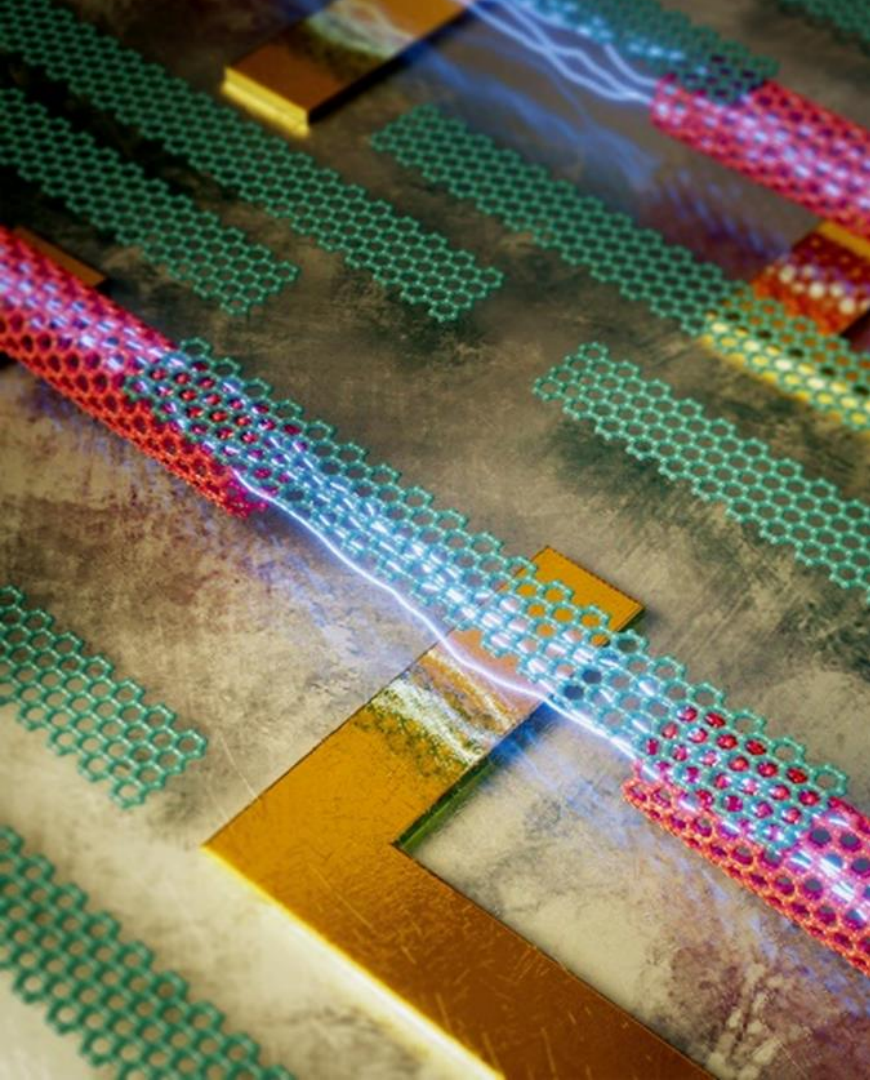
eesa
business
incubation
centre

BRIDGE

Zürcher
Kantonalbank

VENTURE
KICK

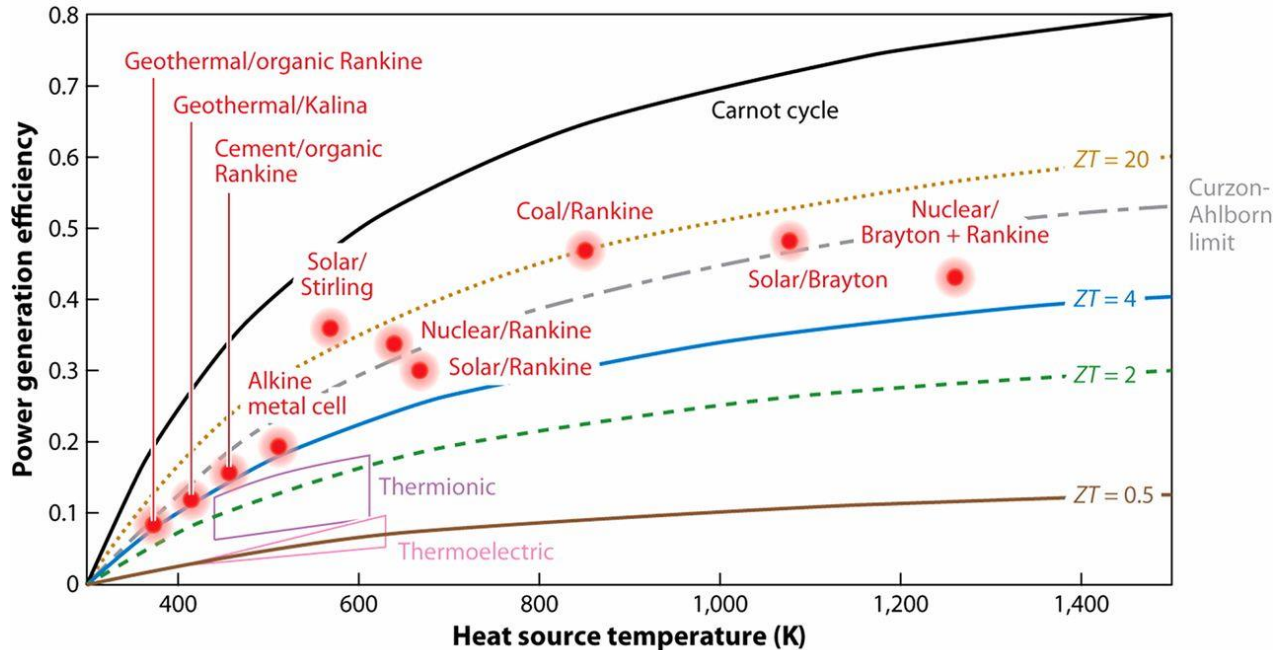
Innosuisse



Quantum heat engines as thermoelectric generators

Generating electricity from (waste) heat?

He et al. Science 2017



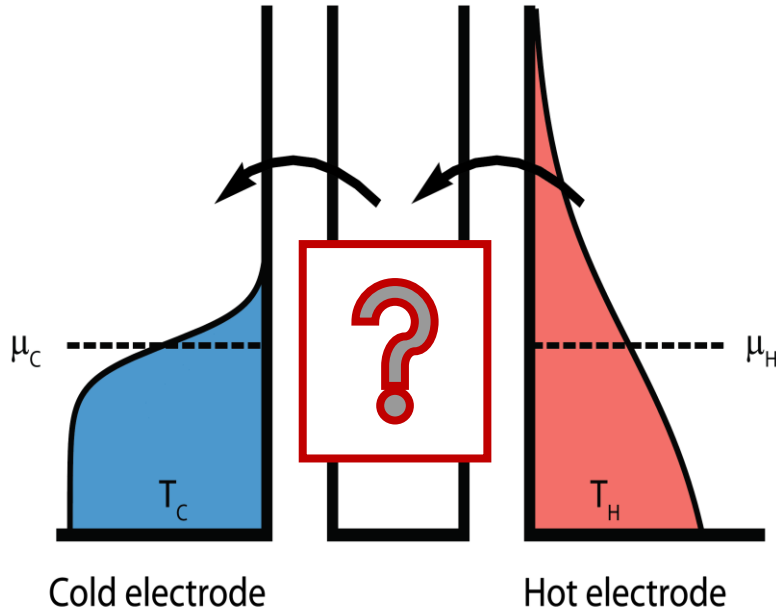
Carnot cycle is upper thermodynamic limit of all heat engines, but no power output is produced

Classical (cyclic) heat engines reach the Curzon-Ahlborn limit of maximum efficiency at maximum power output

Thermoelectrics do not reach Curzon-Ahlborn limit so far!

Can we make thermoelectrics more efficient by using quantum heat engines?

PHE (Particle exchange Heat Engine) Design with electrons



«Quantum dot»

$$\eta = \left(\frac{T_{\text{hot}} - T_{\text{cold}}}{T_{\text{hot}}} \right) \left[\frac{\sqrt{1 + ZT_m} - 1}{\sqrt{1 + ZT_m} + \left(\frac{T_{\text{cold}}}{T_{\text{hot}}} \right)} \right]$$

For $ZT \rightarrow \infty$ $\eta = \left(\frac{T_{\text{hot}} - T_{\text{cold}}}{T_{\text{hot}}} \right)$

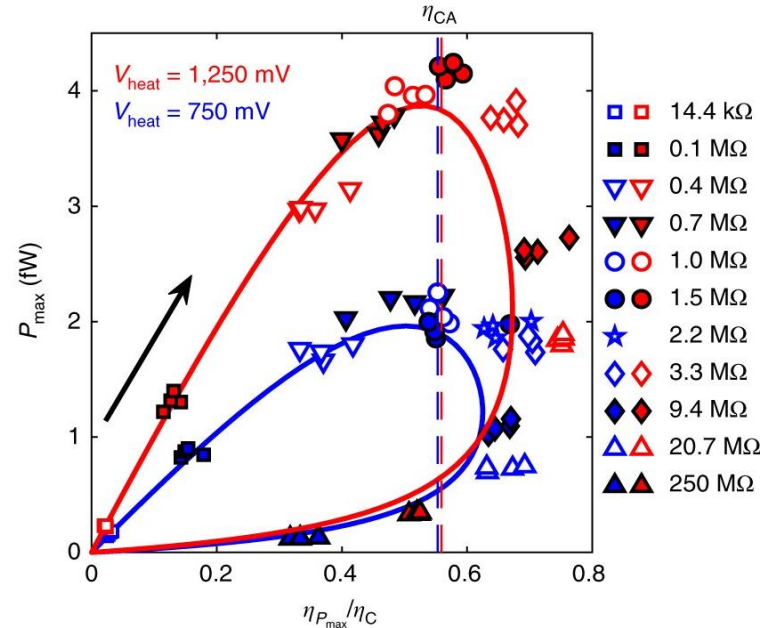
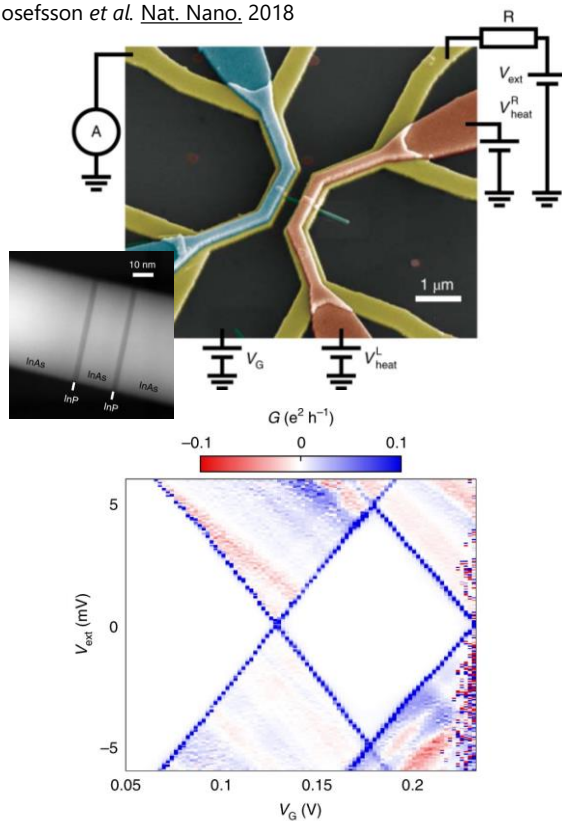
Carnot efficiency

Question: Where is the Curzon-Ahlborn limit for maximum power output?

Experimental quantum heat engine

Curzon-Ahlborn limit

Josefsson et al. Nat. Nano. 2018

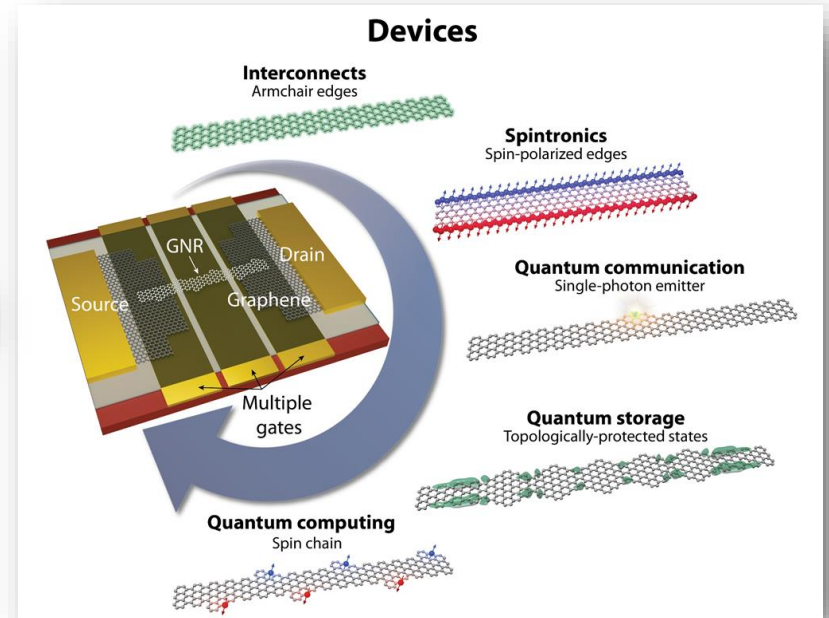
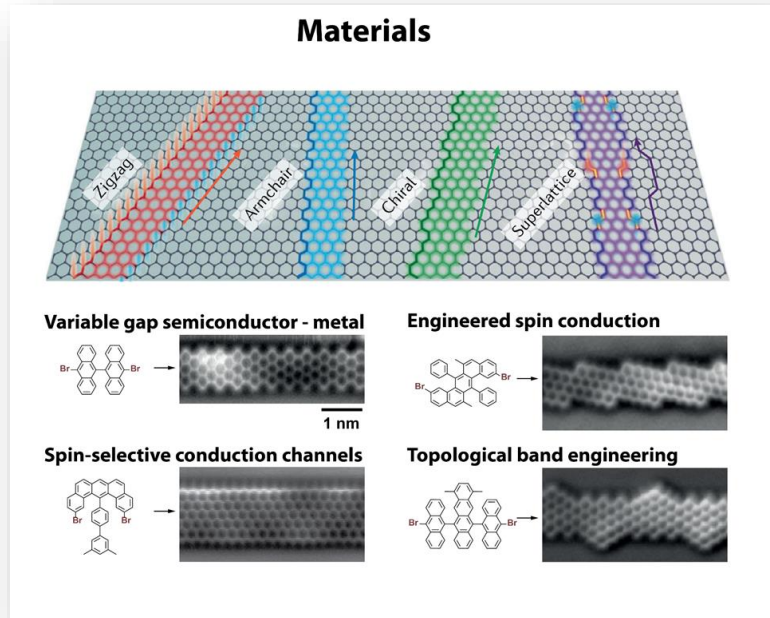


However: This device only operates at temperatures below 1K, level splitting in semiconducting quantum dots is small.

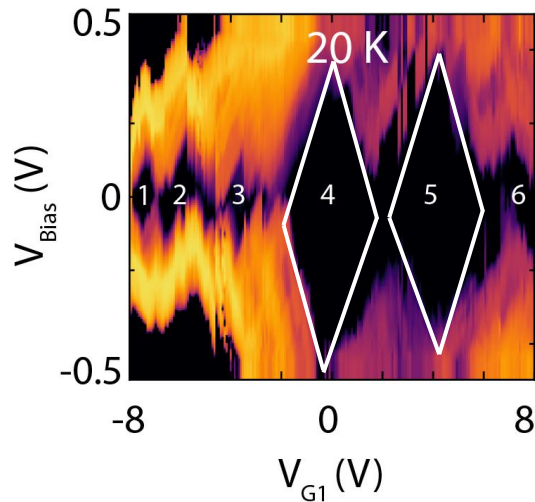
Question: Can we bring up the Quantum Engines to room temperature?

Graphene nanoribbons

A versatile material platform for quantum technologies



Toward room temperature quantum devices



Coulomb diamonds visible up to 250K

Mickal Perrin, ETHZ, Empa, ERC starting grant

Summary

- Physics and chemistry are the base of interdisciplinary, energy-related material science
- Bifacial Solar Cells as way to increase efficiency
- Thin-film batteries strive for high power & energy density at same time
- Exploratory new methods like quantum heat engines are at the horizon as a new generation of thermoelectric generators.

Empa – The Place where Innovation Starts

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Materials Science and Technology

