



# Estimating the Background Potential of Quantum Constrictions Using Scanning Gate Microscopy and Machine Learning

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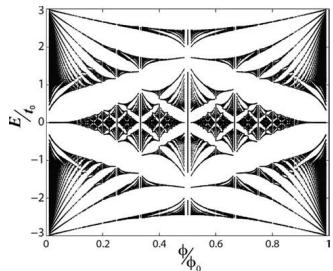
<sup>3</sup> Department of Electronics, Chiba University, Japan

65<sup>th</sup> Electronic Materials Conference  
Nanoscale Characterization – June 28<sup>th</sup>



# Quantum Materials

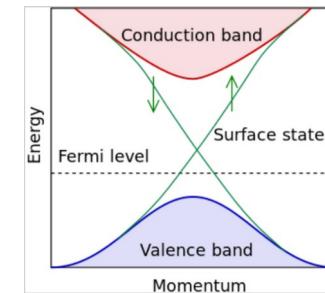
Quantum Hall



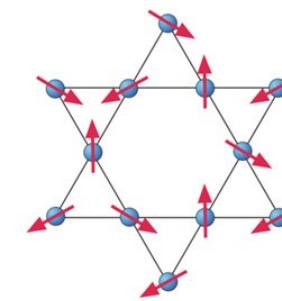
Superconductivity



Topological insulators

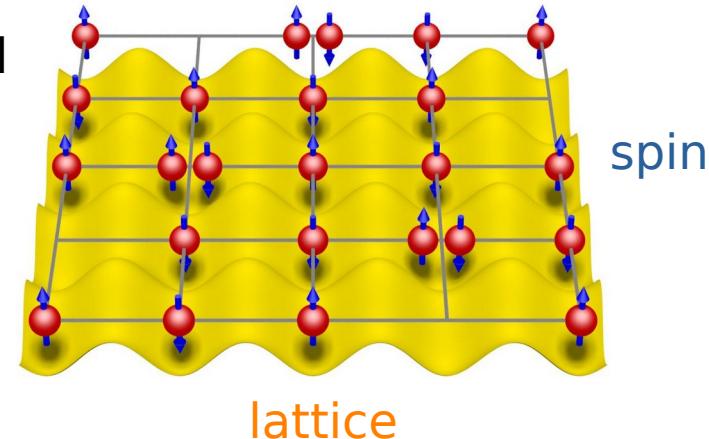


Spin liquids



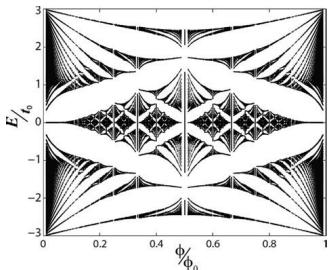
orbital

charge



# Quantum Materials

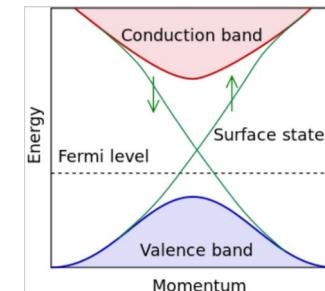
Quantum Hall



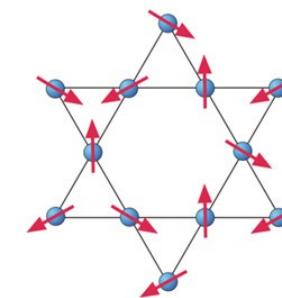
Superconductivity



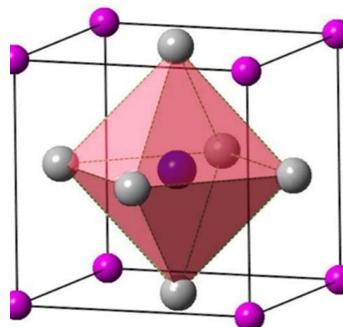
Topological insulators



Spin liquids

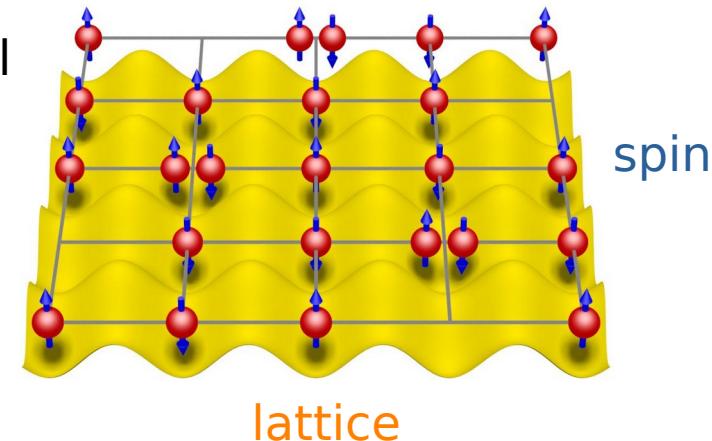


$\text{Bi}_2\text{Te}_3$

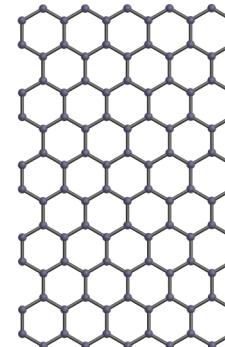


orbital

charge



Graphene



# Quantum Materials

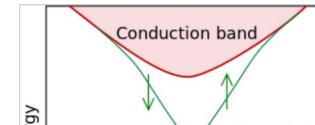
Quantum Hall



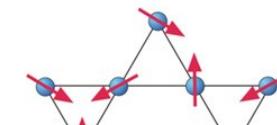
Superconductivity



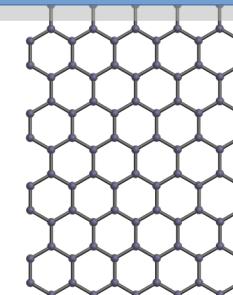
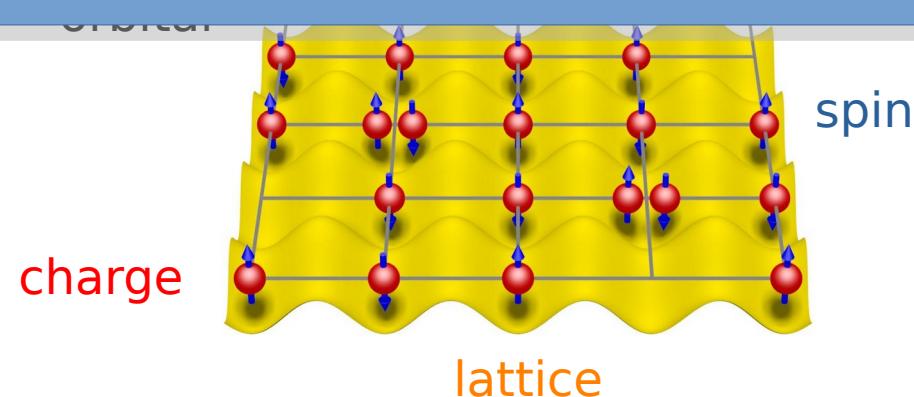
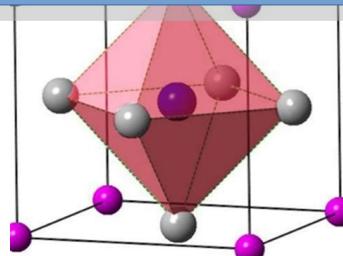
Topological insulators



Spin liquids

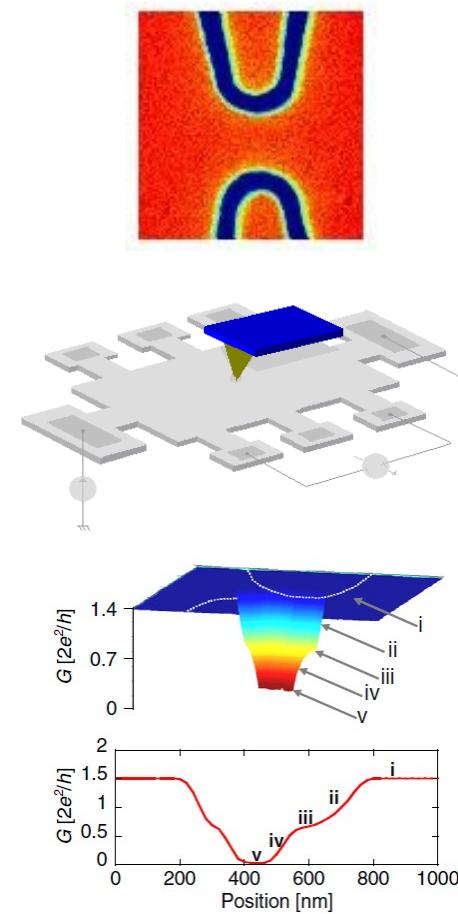


Defects play a major role!

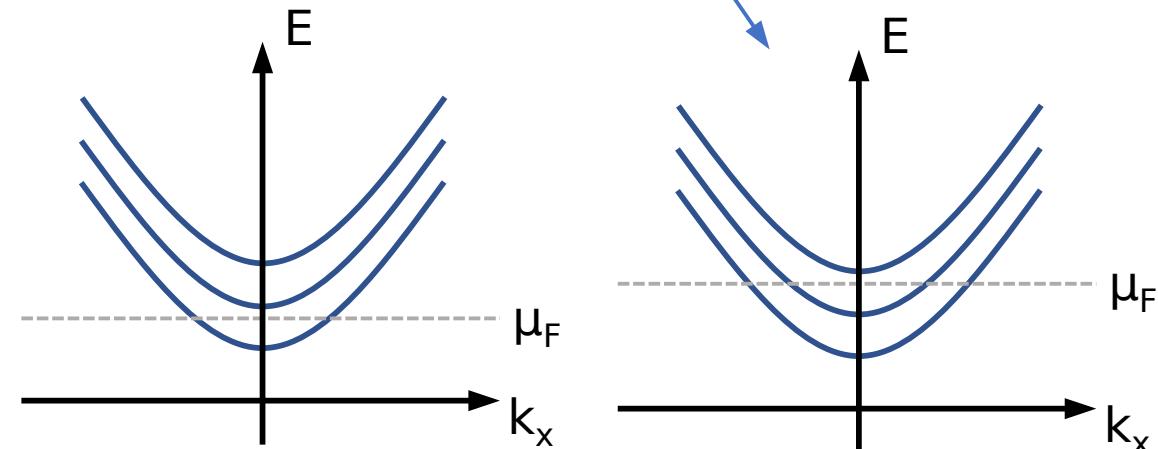
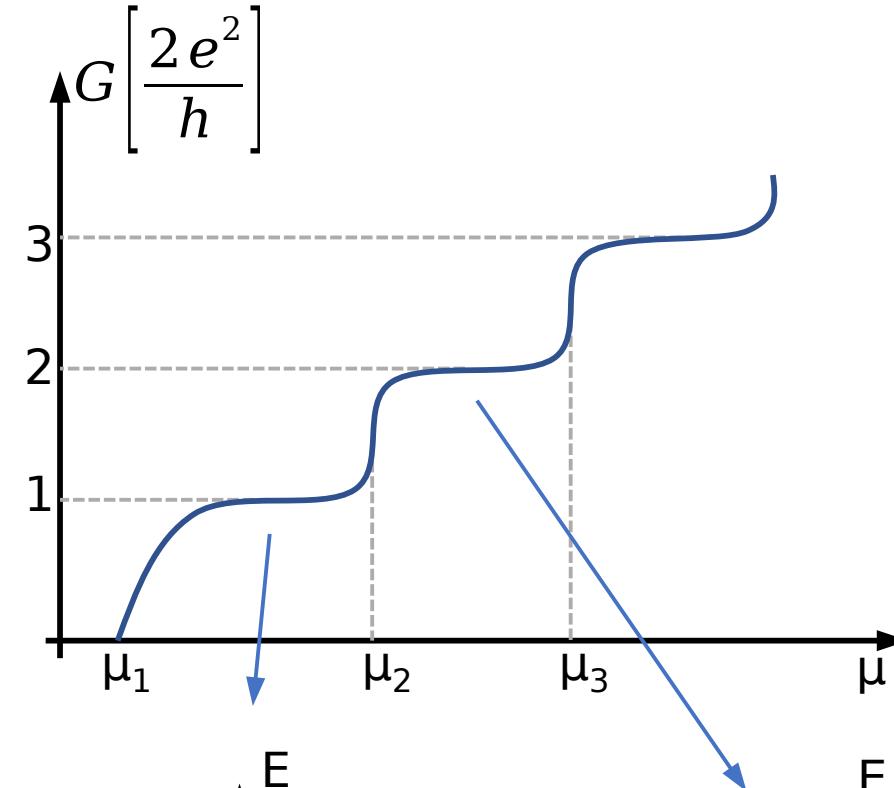
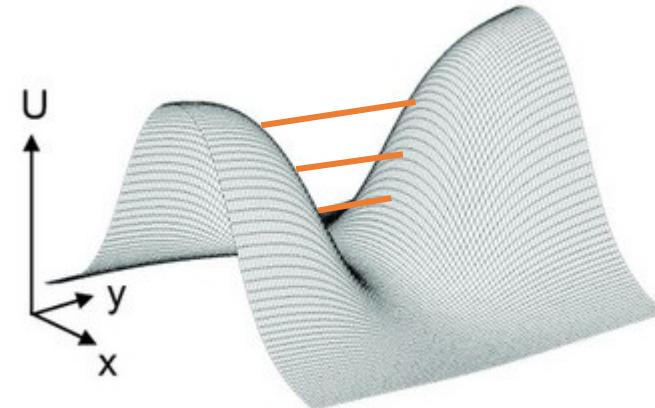
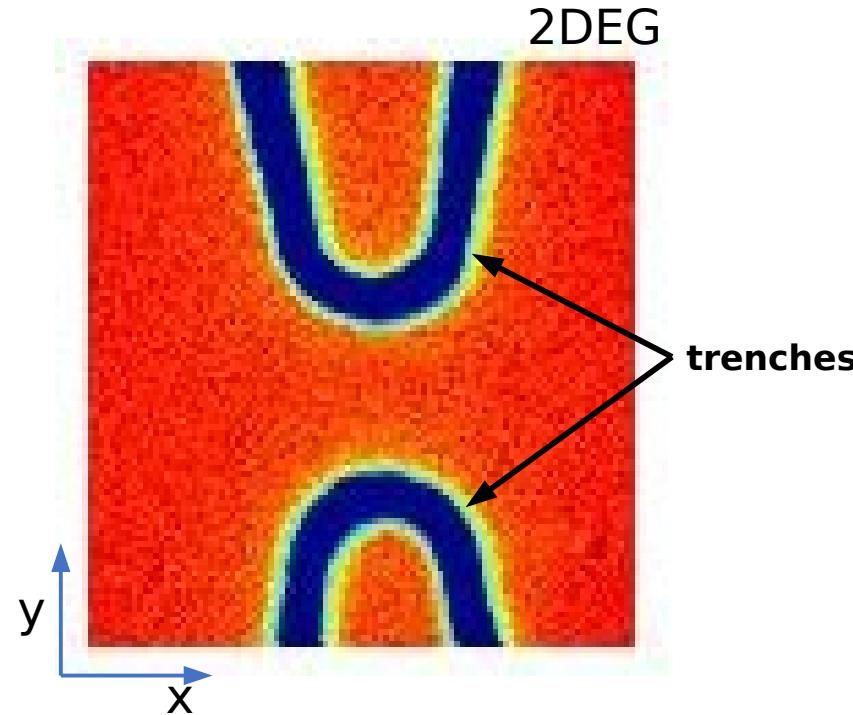


# Structure of the Talk

- Quantum Point Contacts (QPC)
- Scanning Gate Microscopy (SGM)
- Device Fabrication
- Characterization
  - Transmission
  - Shubnikov-de Haas
  - SGM
- Machine Learning
  - Convolutional Neural Nets
  - Cellular Neural Nets
- Stigmergy Meta-Heuristics
  - Roughness
  - Correlations
- Conclusions



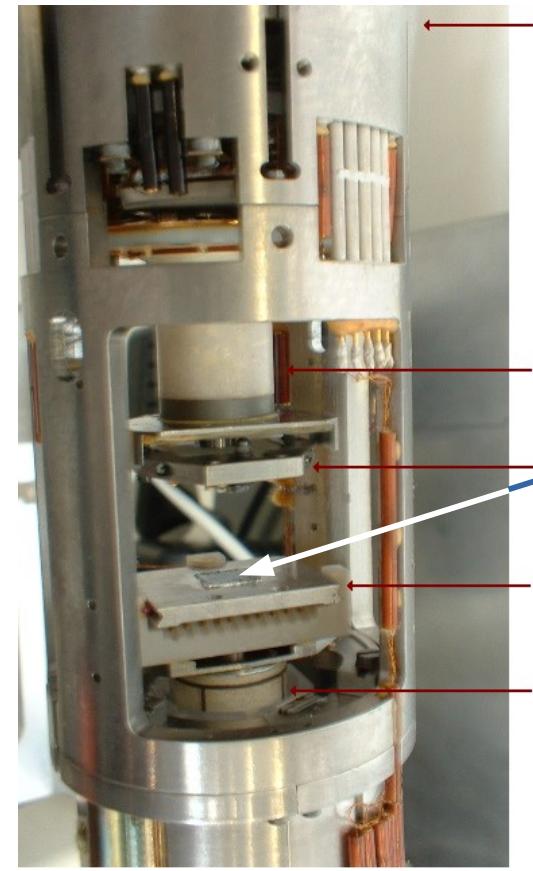
# Quantum Point Contacts



Bart Van Wees  
(U. Groningen - Netherlands)

B.J. van Wees et al. "Quantized conductance of point contacts in a two-dimensional electron gas". *Phys. Rev. Lett.* **60**-9 (1988) 848–850.

# Scanning Gate Microscopy



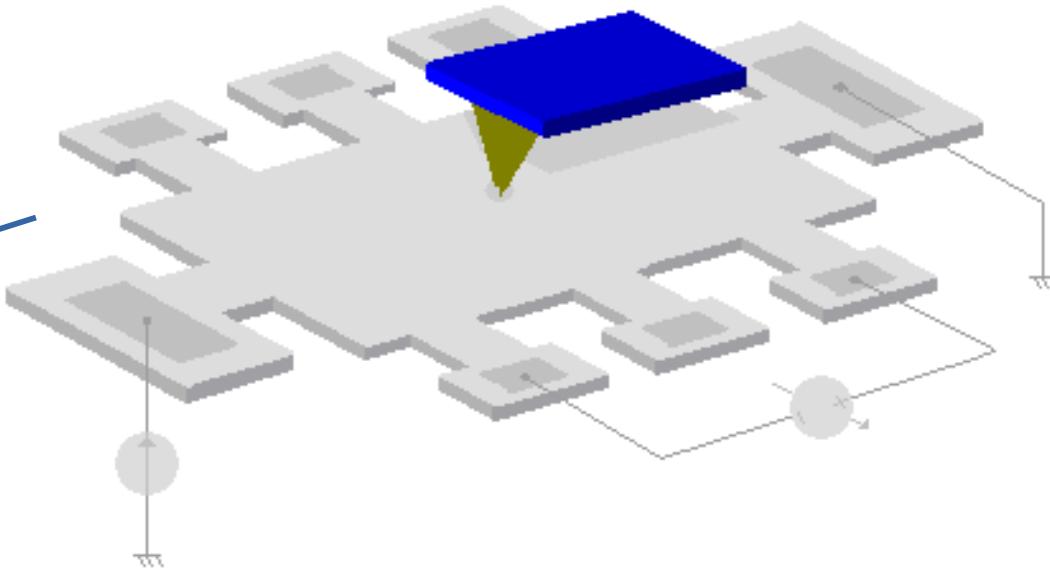
Electrical Contacts

Non-contact piezo

Cantilever stage

Sample stage

X-Y-Z Tube Scanner  
with Picomotor



$$E_n \approx E_n^0 + \langle n | V | n \rangle$$

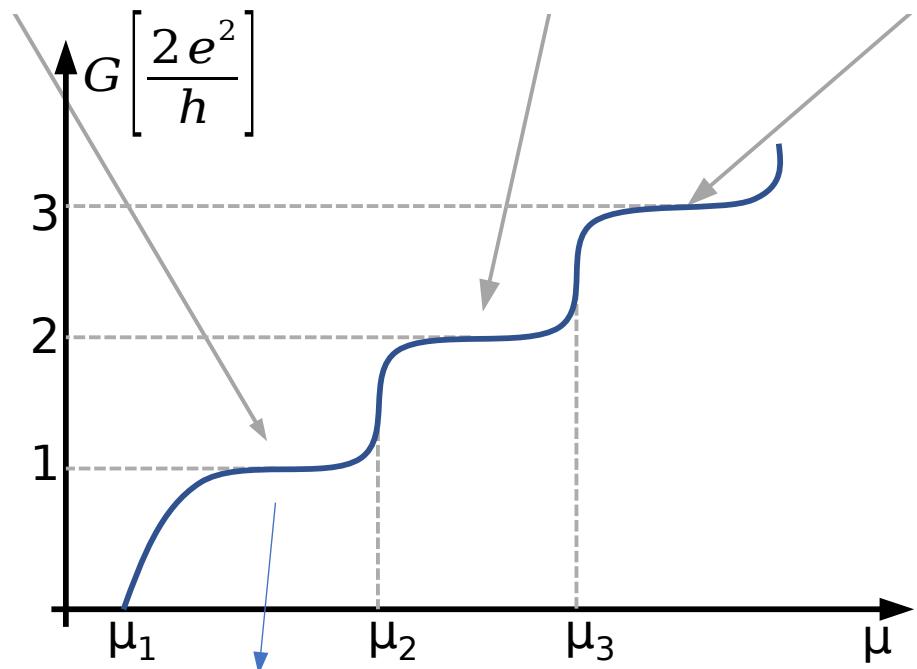
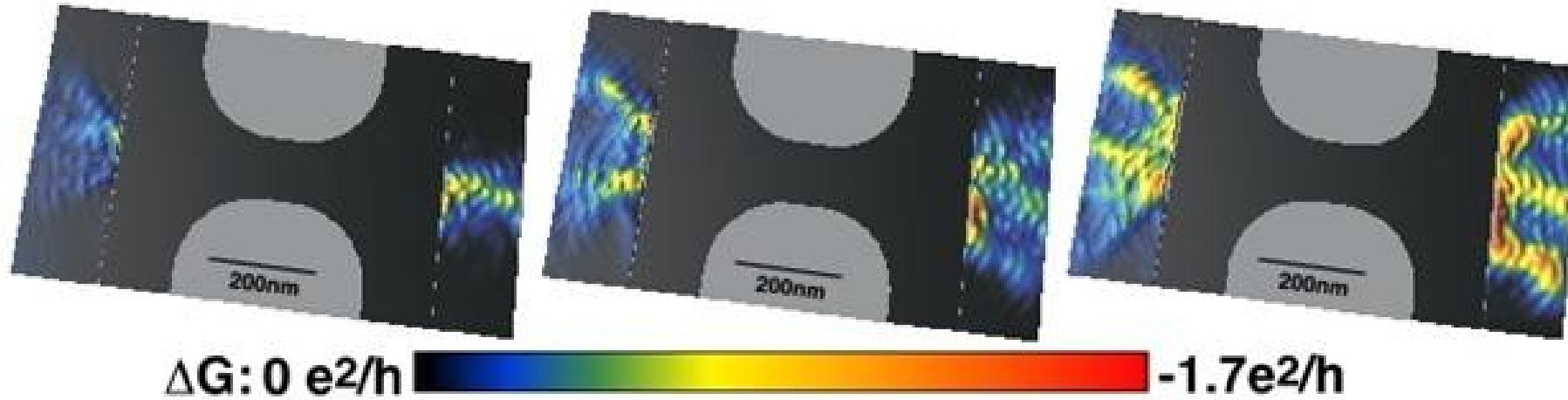
$$\Delta E_n \approx V_0 |\varphi_n(\mathbf{r}_0)|^2$$

Shifts proportional to LDOS

$$\Delta G(\mathbf{r}_0) \approx \frac{\partial G}{\partial E_F} \Delta E_n$$

$$\Delta G(\mathbf{r}_0) \approx V_0 \frac{\partial G}{\partial E_F} |\varphi_n(\mathbf{r}_n)|^2$$

# Electron Flow

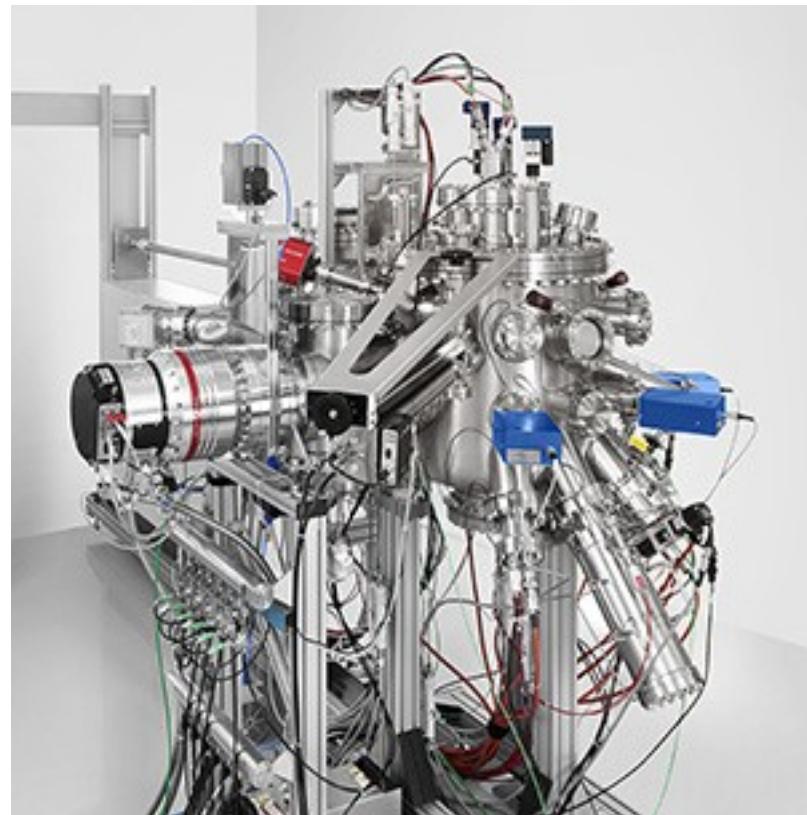
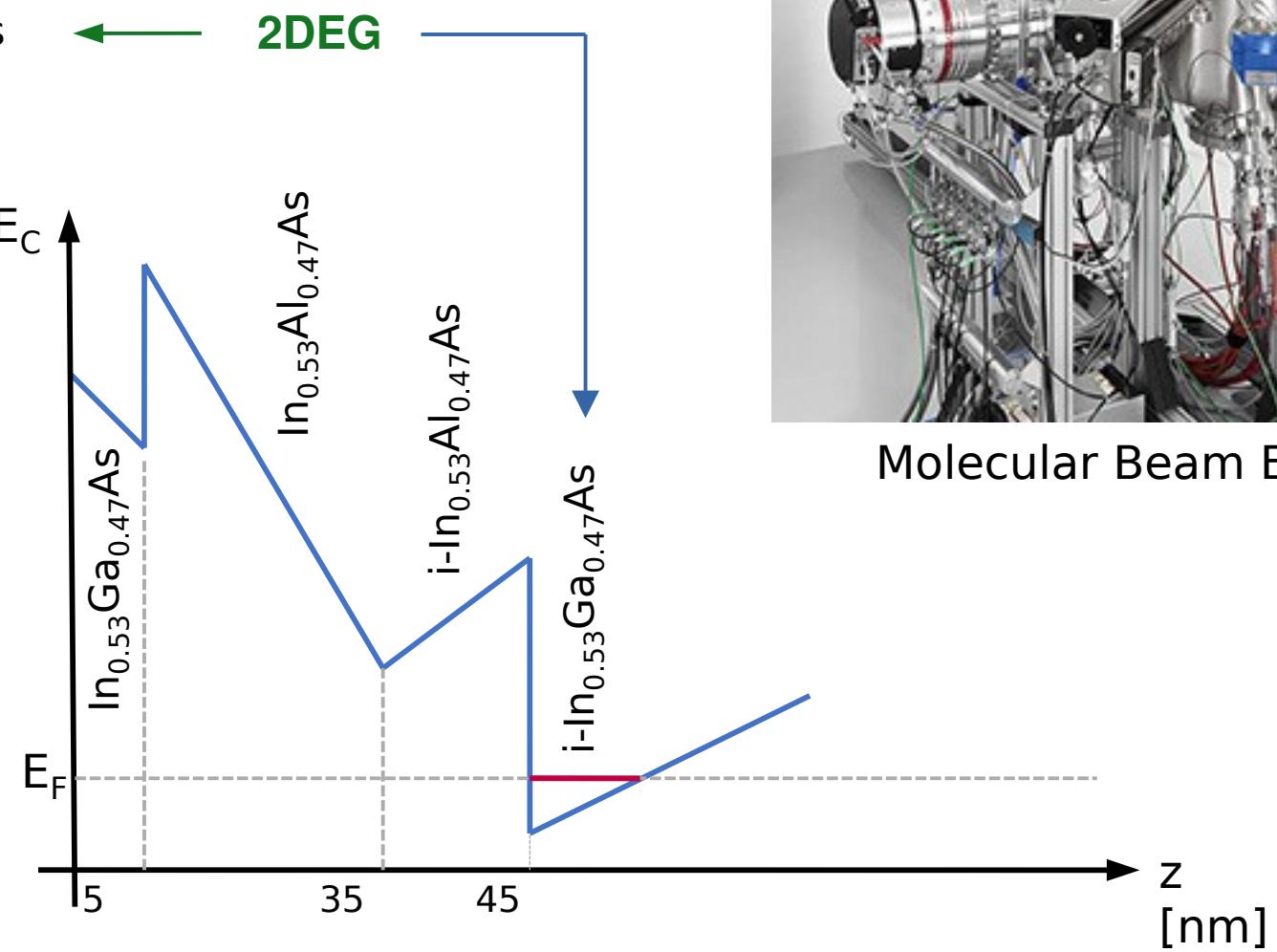
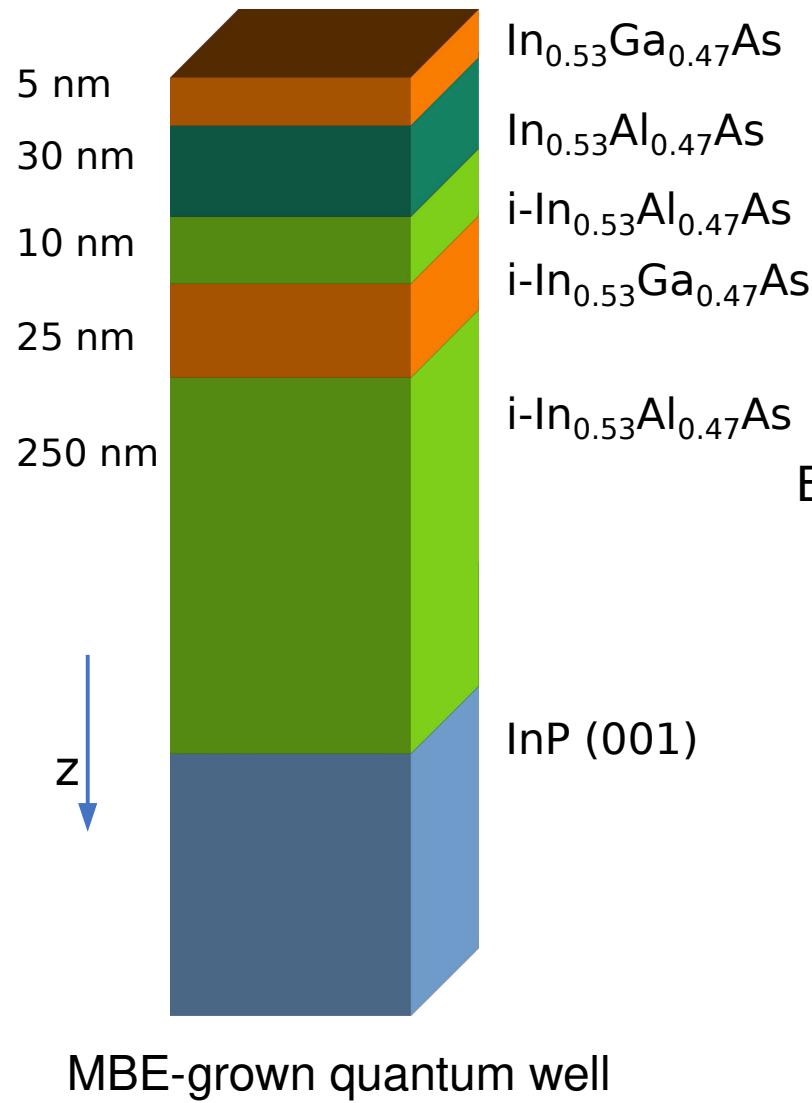


R. Westervelt  
(Harvard)

M. A. Topinka, B. J. LeRoy, S. E. J. Shaw, E. J. Heller, R. M. Westervelt, K. D. Maranowski, A. C. Gossard, "Imaging Coherent Electron Flow from a Quantum Point Contact", *Science* **289** (2000) 2323.

# Device Fabrication

## Heterostructure



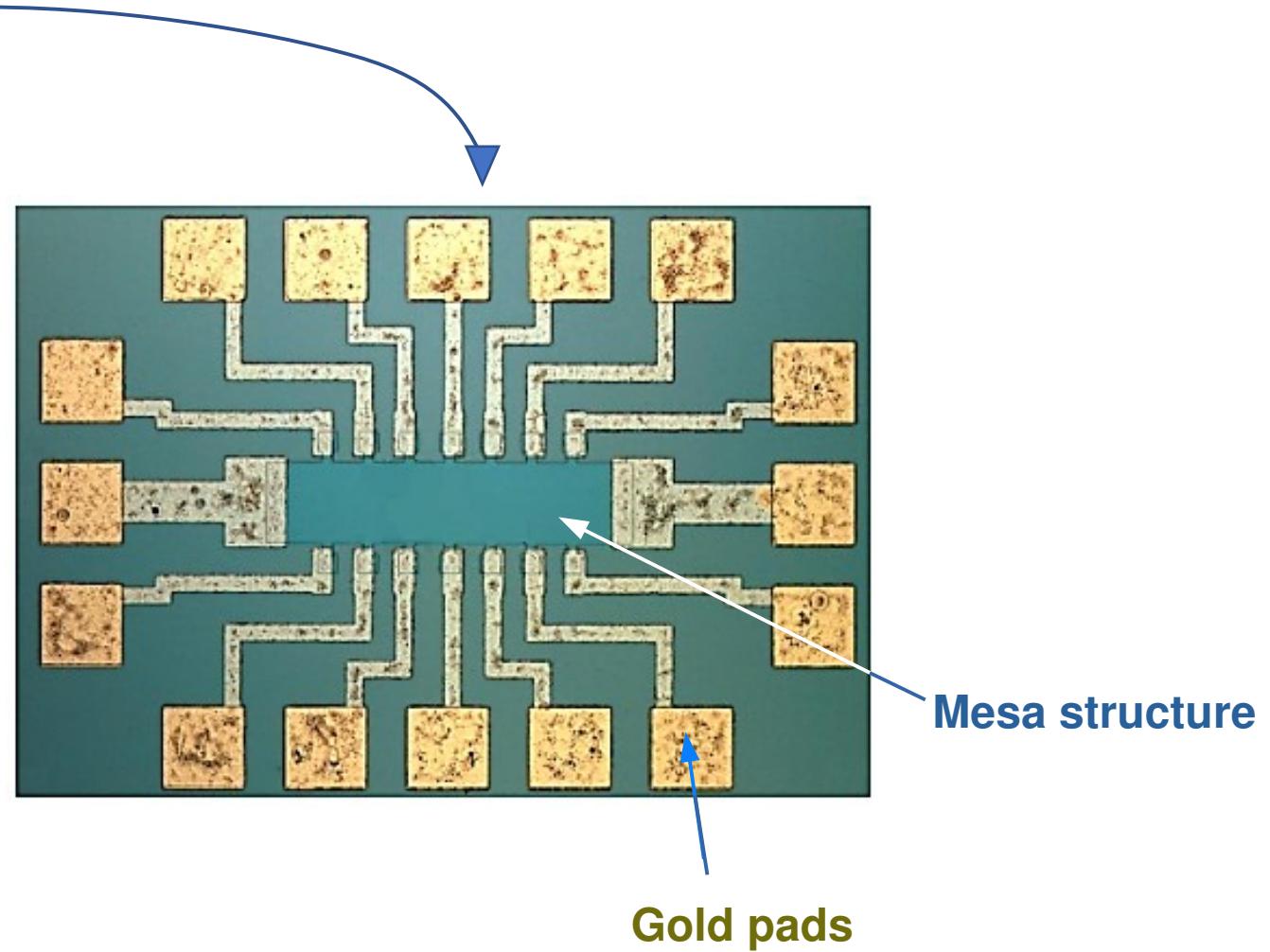
Hall bar

5 nm  
30 nm  
10 nm  
25 nm  
250 nm

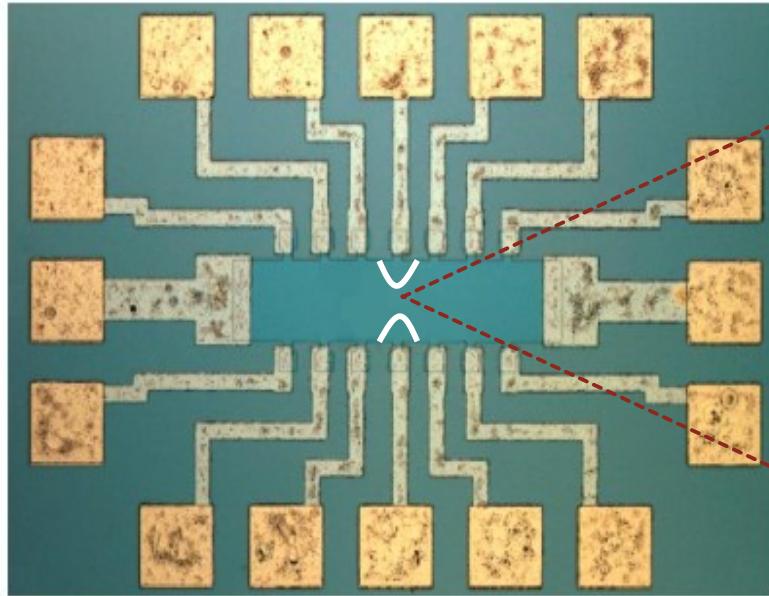
$\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$   
 $\text{In}_{0.53}\text{Al}_{0.47}\text{As}$   
i- $\text{In}_{0.53}\text{Al}_{0.47}\text{As}$   
i- $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}$   
i- $\text{In}_{0.53}\text{Al}_{0.47}\text{As}$   
InP (001)

z

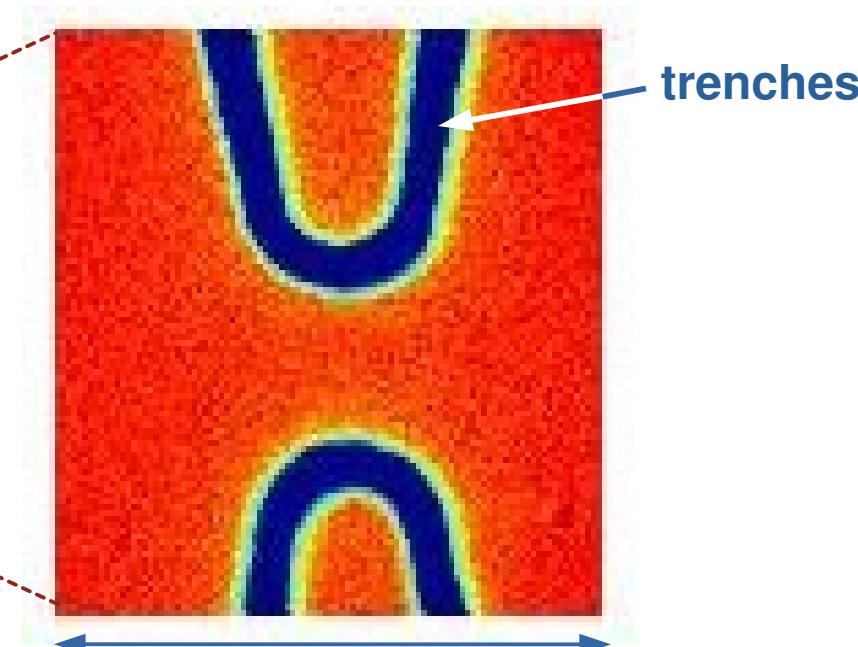
MBE-grown quantum well



## EBL-Defined QPC



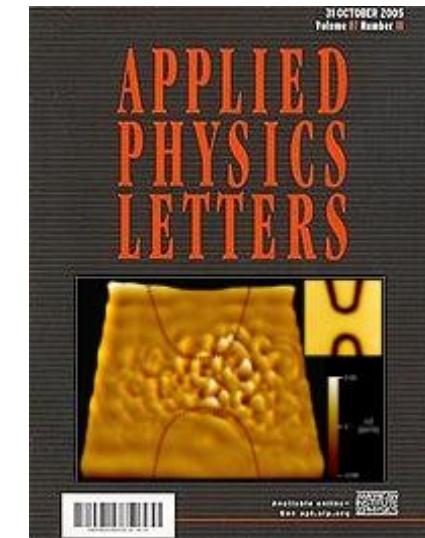
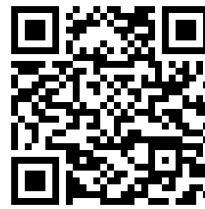
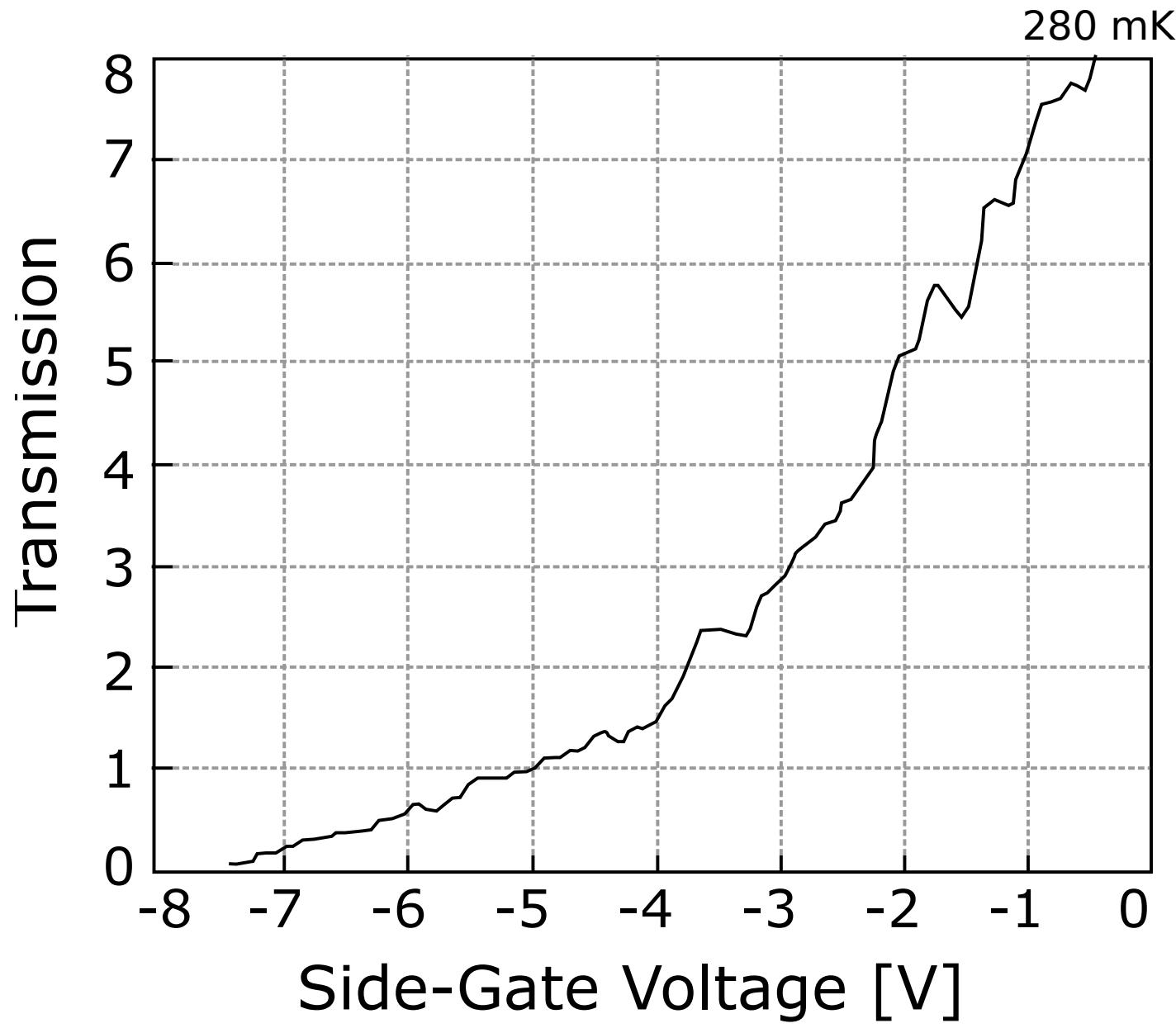
Electron beam lithography



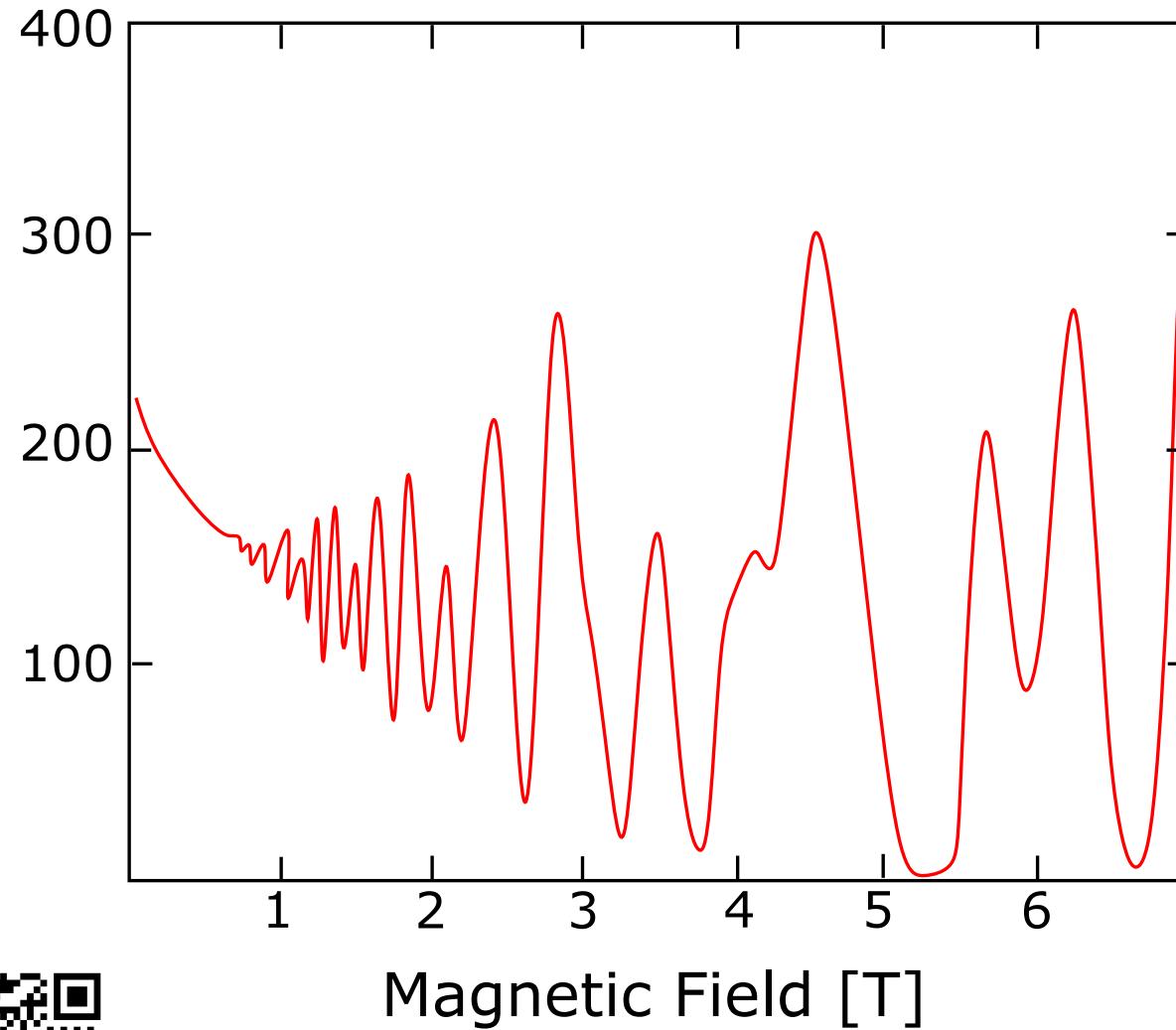
# Characterization

- Shubnikov de-Haas
- Quantum Hall
- Quantum Chaos

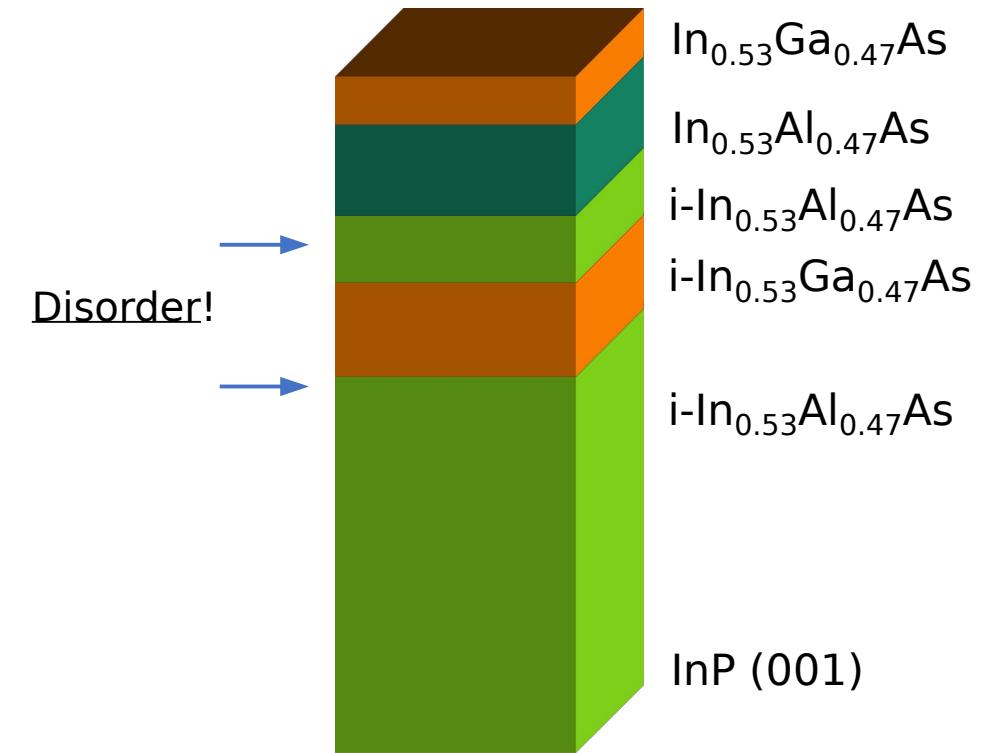
# Transmission



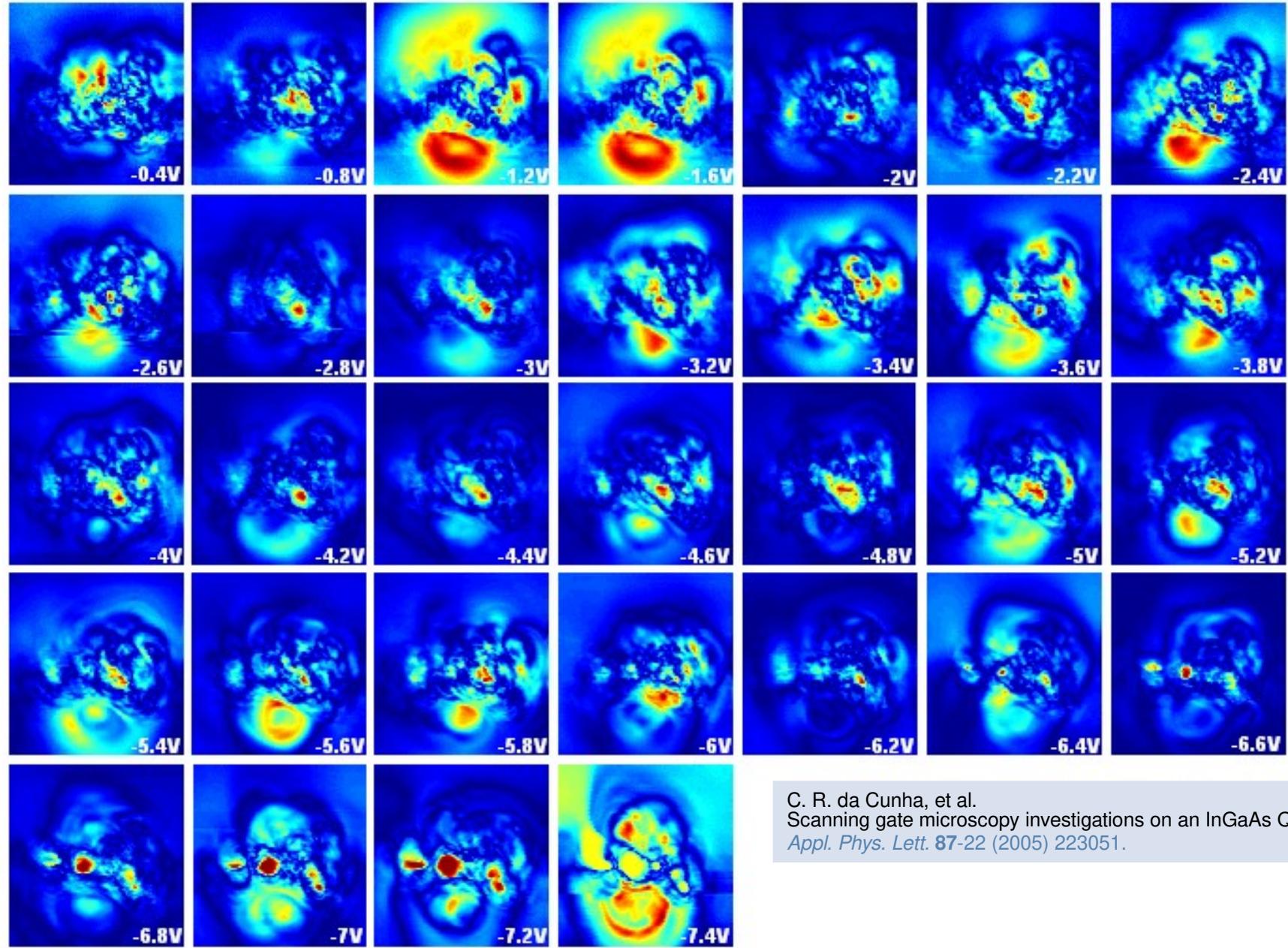
C. R. da Cunha, et al.  
Imaging of quantum interference patterns within a quantum  
point contact  
*Appl. Phys. Lett.* **89-24** (2006) 242109.



$n = 7.2 \times 10^{11} \text{ cm}^{-2}, 2.1 \times 10^{11} \text{ cm}^{-2}$   
 $\mu = 7.4 \times 10^4 \text{ cm}^2/\text{V.s}$   
 $l = 1.2 \mu\text{m}$



# Scanning Gate Microscopy



C. R. da Cunha, et al.  
Scanning gate microscopy investigations on an InGaAs QPC  
*Appl. Phys. Lett.* **87-22** (2005) 223051.



# IF {

1. The perturbation is sufficiently small;
2. The induced potential is delta-shaped
3. Wave function is given solely by states at the Fermi energy;
4. The conductance does not change much with Fermi energy (plateau);

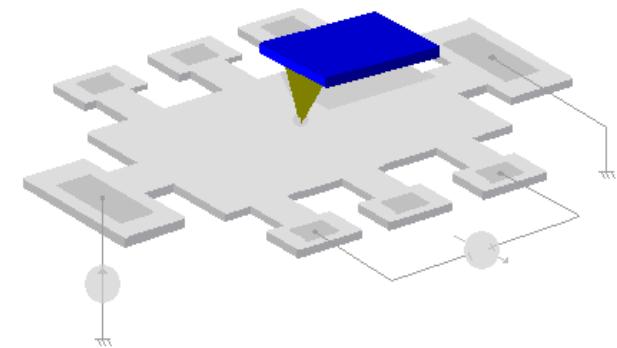
# }

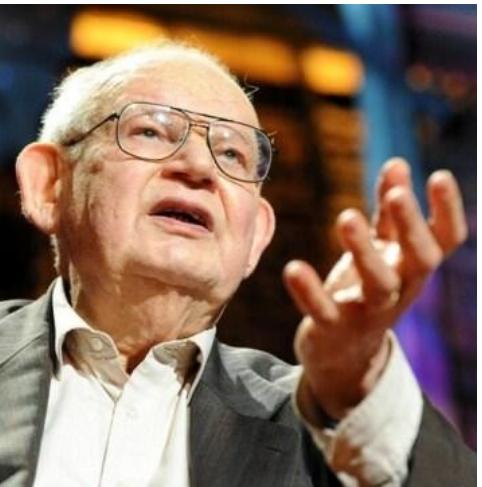
# Then {

Changes in conductance ( $\Delta G$ )  $\propto$  local density of states (LDOS).

$$\Delta G(\mathbf{r}_0) \approx V_0 \frac{\partial G}{\partial E_F} |\varphi_n(\mathbf{r}_n)|^2$$

# }





B. Mandelbrot  
(1924 – 2010)

# But...

Clouds are not spheres, mountains are not cones, coastlines are not circles, barks are not smooth, lighting does not travel in a straight line,...

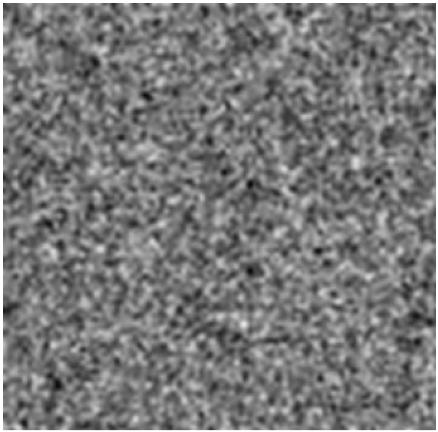
...  $\Delta G$  is not small, the tip potential is not delta-shaped, not all states are in the Fermi level, and the conductance changes considerably with the Fermi level.



# Machine Learning

- Cellular Neural Networks
- Stigmergy Meta-heuristics

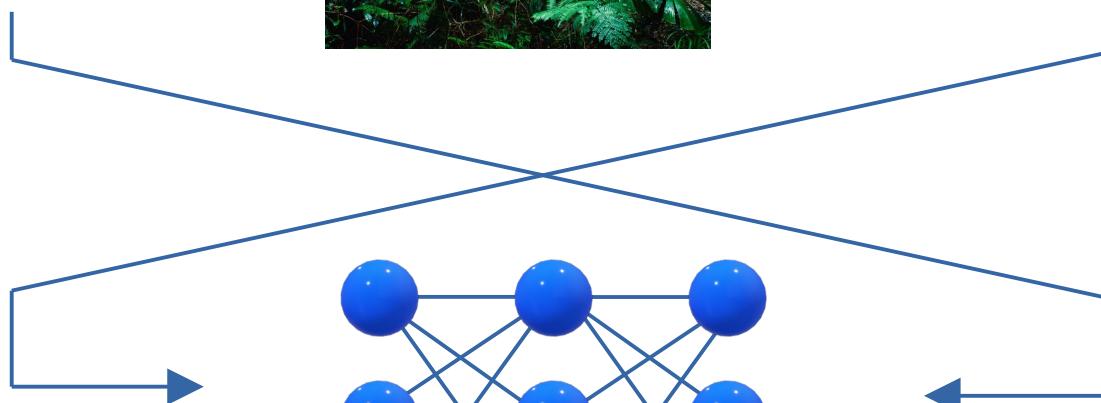
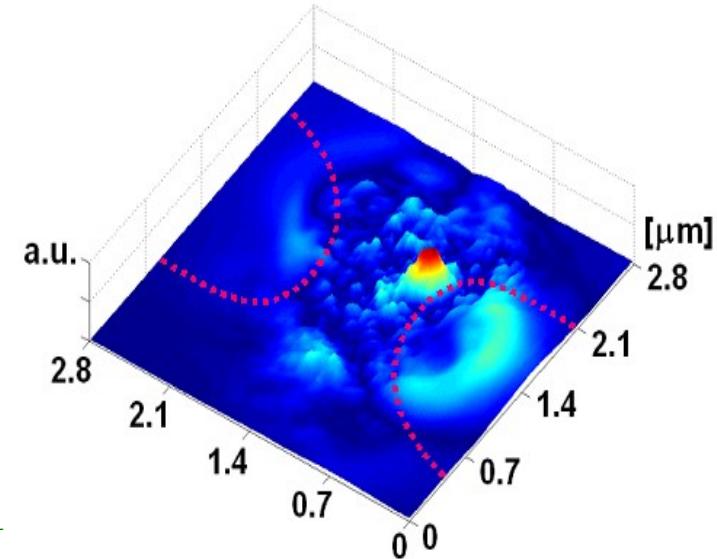
# Inverse Problem



Random Potentials



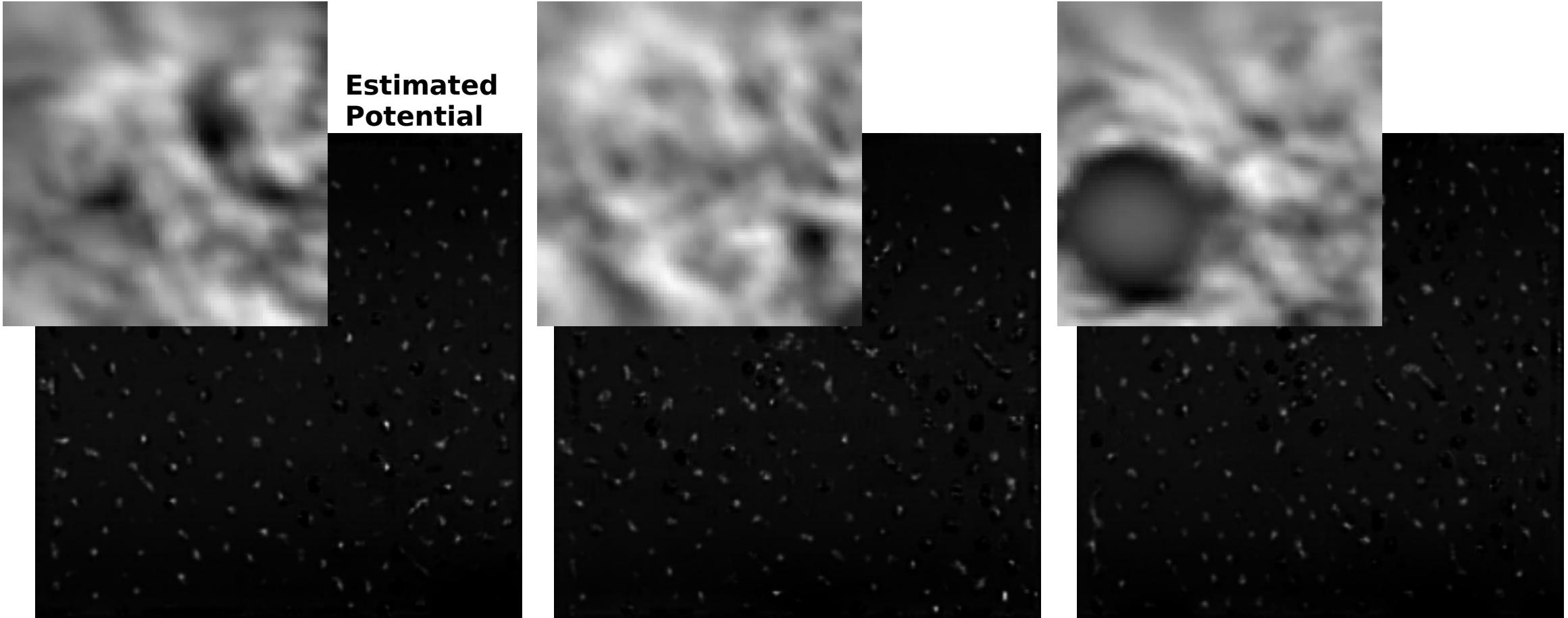
$$G_{nn}^0(E) = [(E + i\eta)I - H_n]^{-1}$$



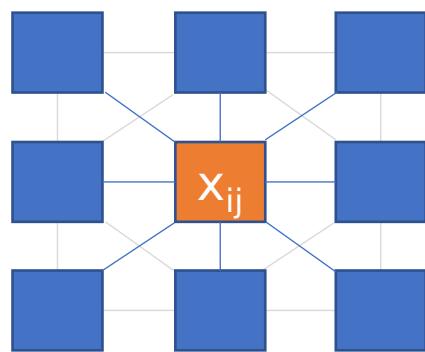
Nonlinear array of elements

## Results

### SGM



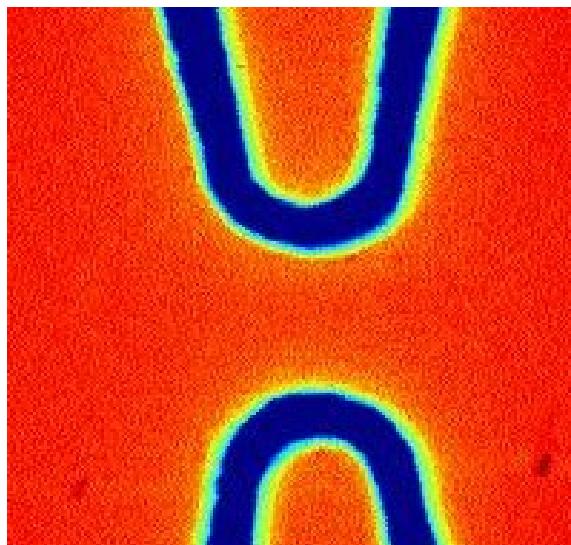
Slow processing limits the number of training samples!



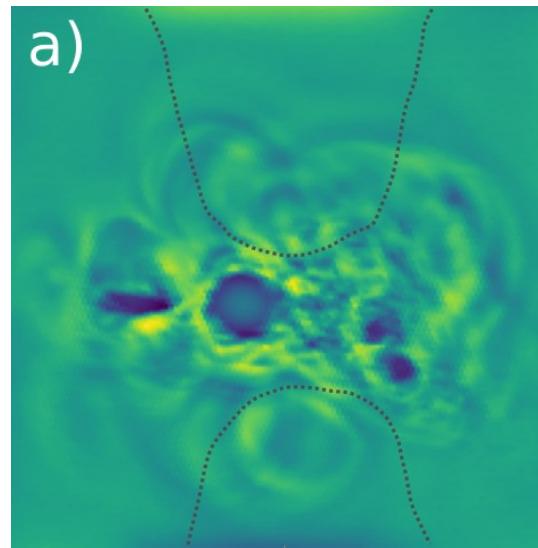
$$\frac{dX_{i,j}(t)}{dt} = -X_{i,j}(t) + \sum_{k,l} A_{i,j,k,l} Y_{k,l}(t) + \sum_{k,l} B_{i,j,k,l} U_{k,l}(t) + Z$$

↑ state                      ↑ output                      ↑ input

Theoretical Potential



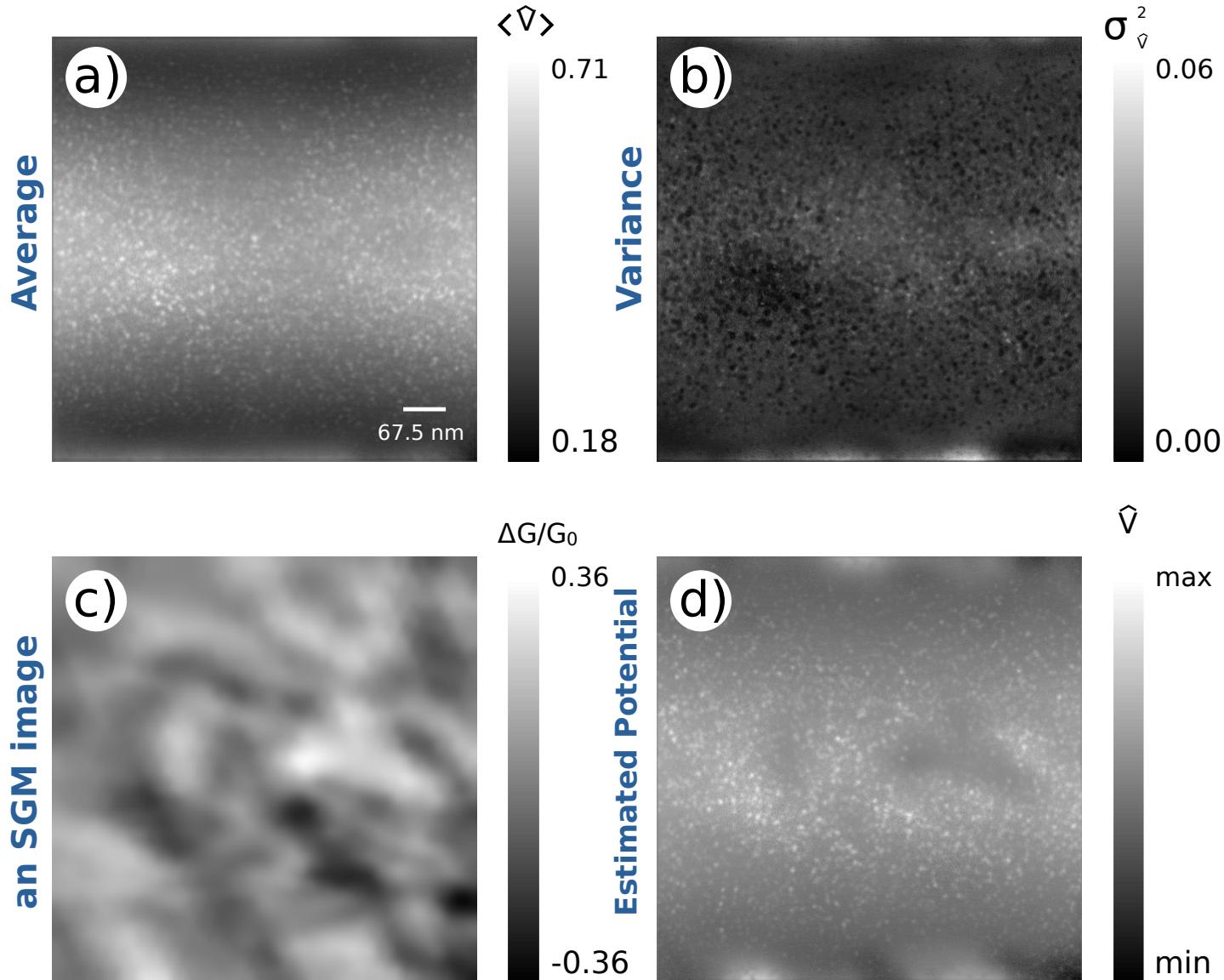
Theoretical LDOS



10k pairs with  
random Gaussian  
noise.

CNN  $\equiv$  Dynamical System. Attractor:  $X(t \rightarrow \infty)$

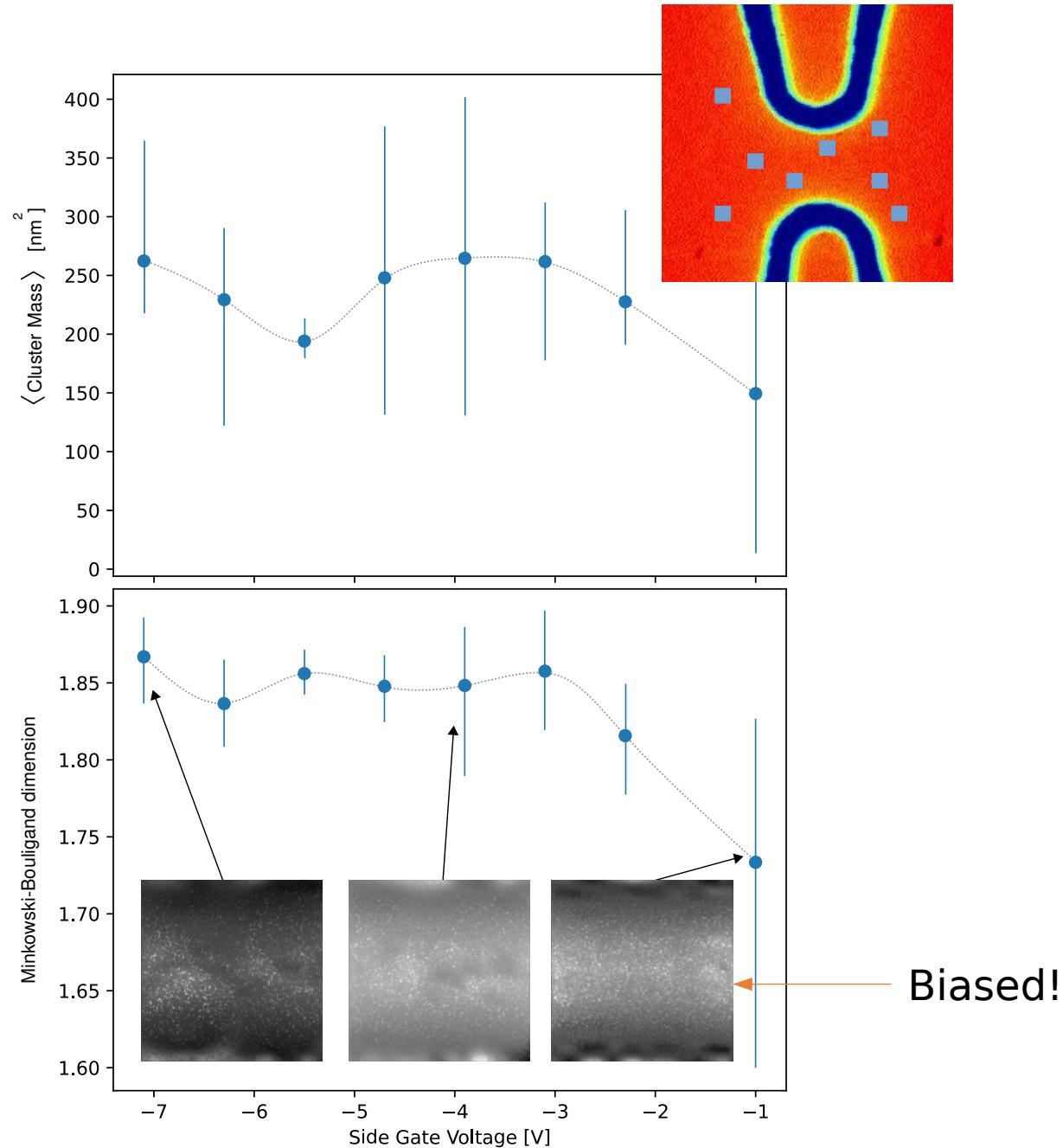
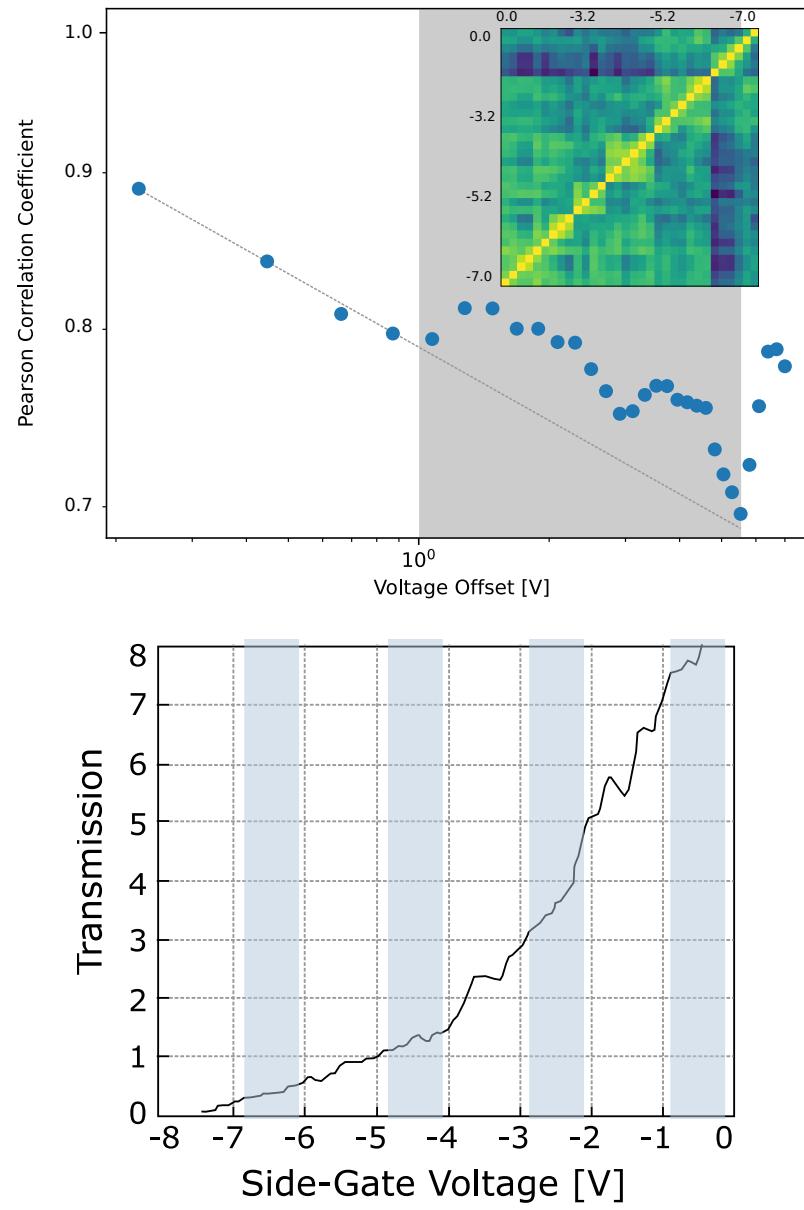
## Results



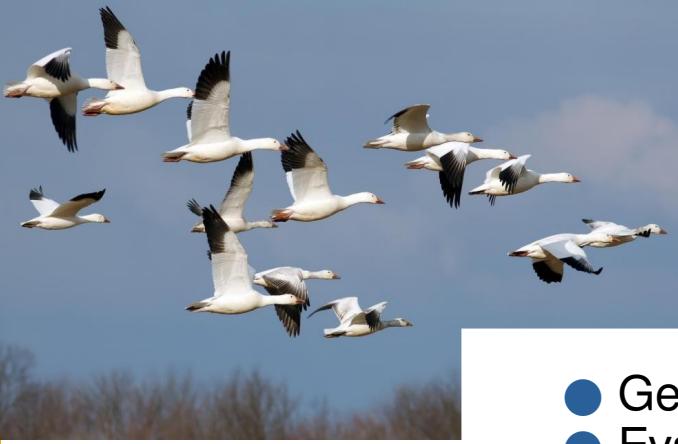
C. R. da Cunha, et al. A method for finding the background potential of quantum devices from scanning gate microscopy data using machine learning, *Mach. Learn. Sci. Tech.* **3** (2022) 025013.



# Statistics



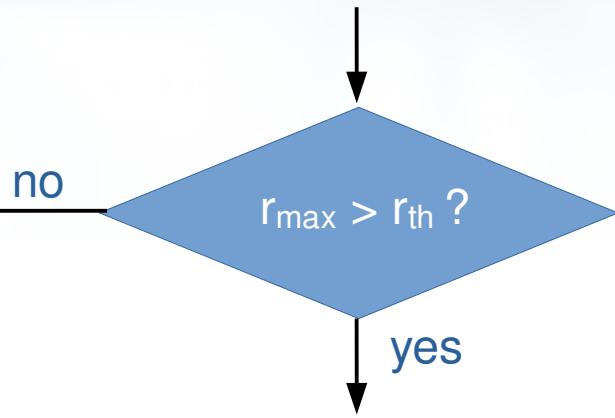
# Stigmergy Meta-Heuristics

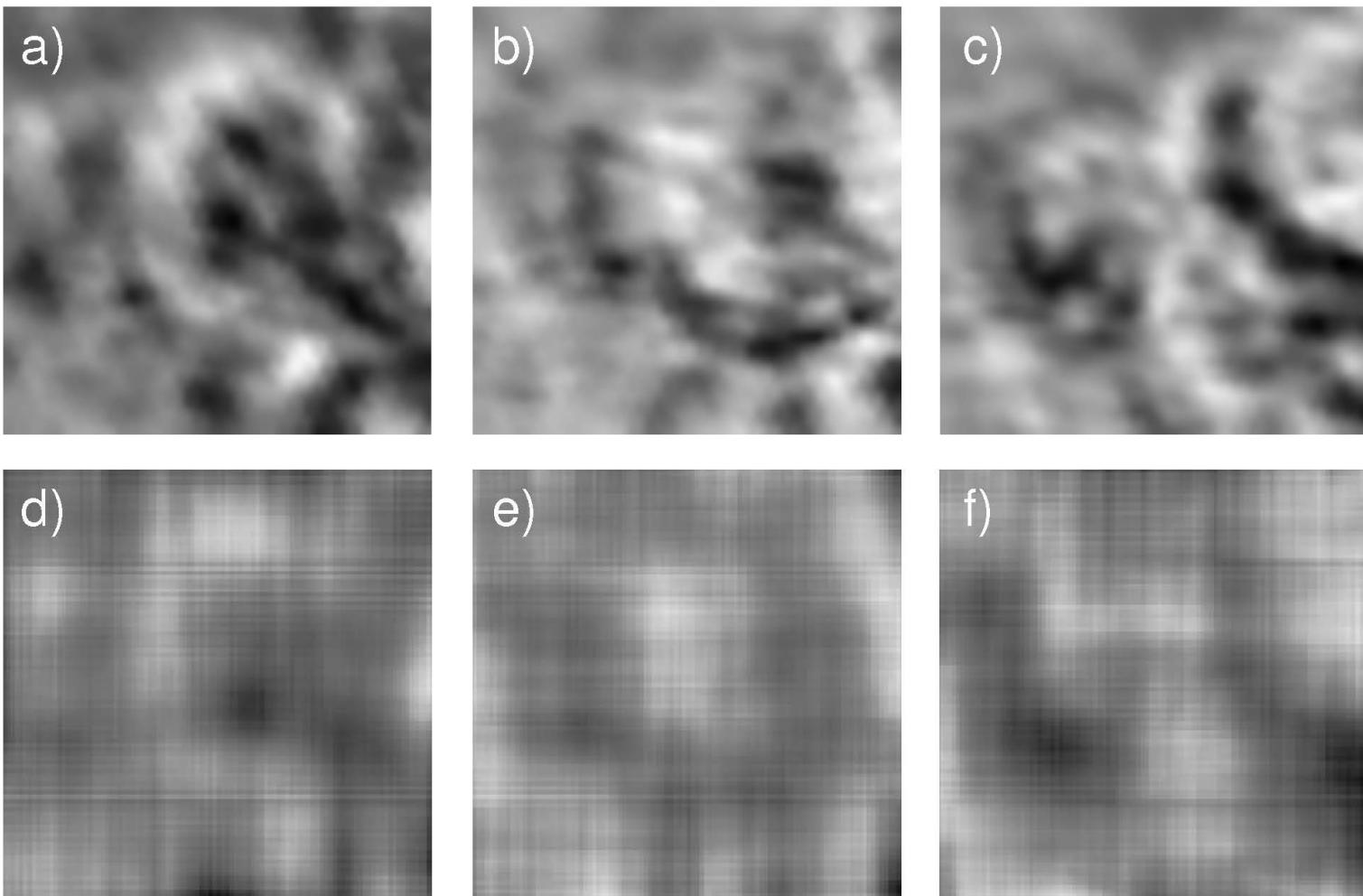


- Generate random population (potentials  $\mu$ );
- Evaluate LDOS' via [Green's functions](#);
- Get rewards  $r$  for all individuals (correlation with expected LDOS);
- Relax all individuals towards the one with the highest reward and add noise:

$$\frac{d \mu(r, t)}{dt} = -\frac{\mu(r, t) - \mu_{max}}{\tau} + \theta(r) \eta \rightarrow \text{Gaussian noise}$$

$\mu_0 e^{-\gamma r}$  High rewards, less noise

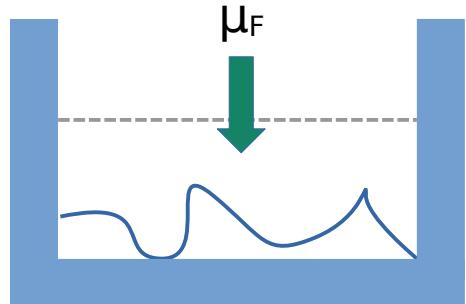
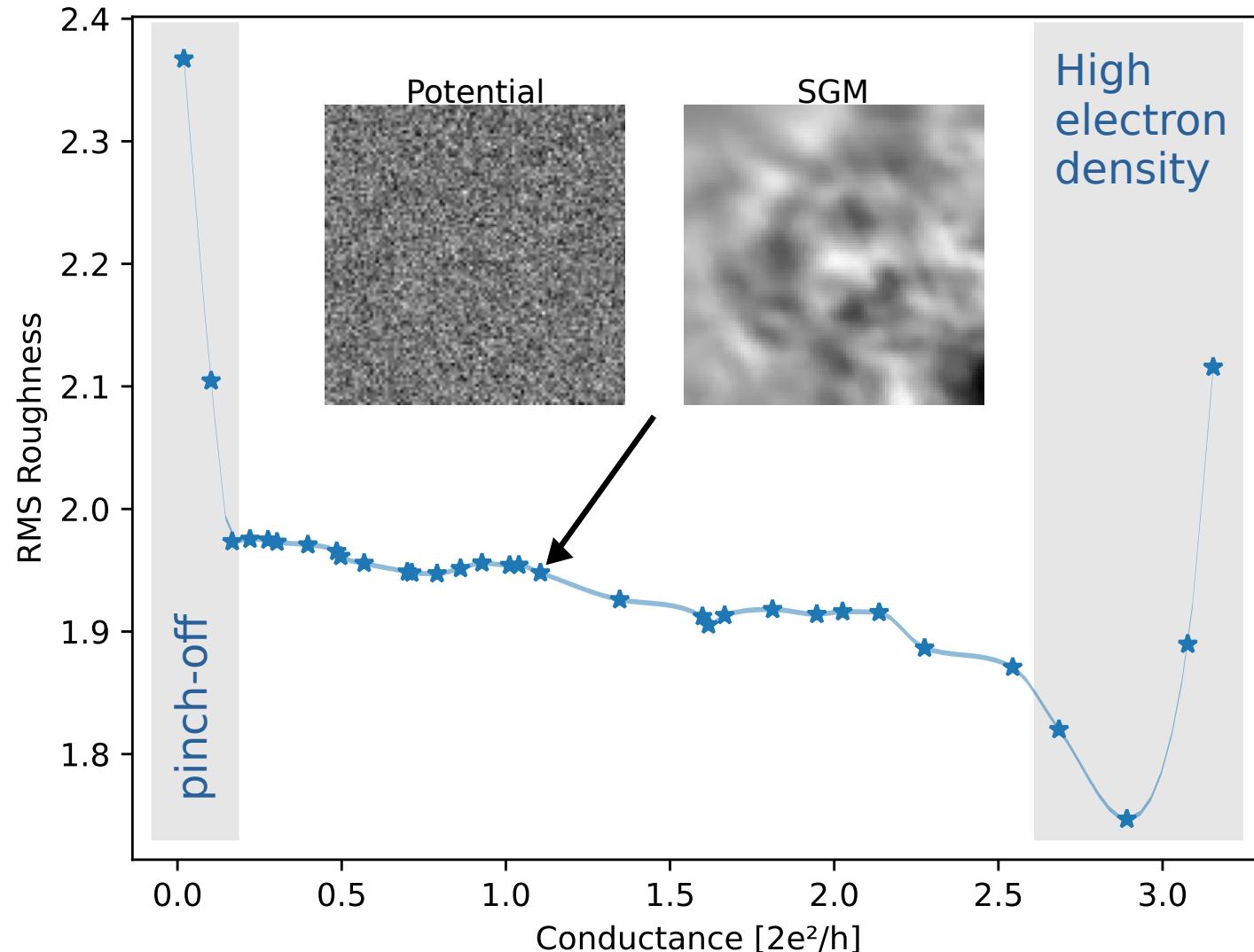




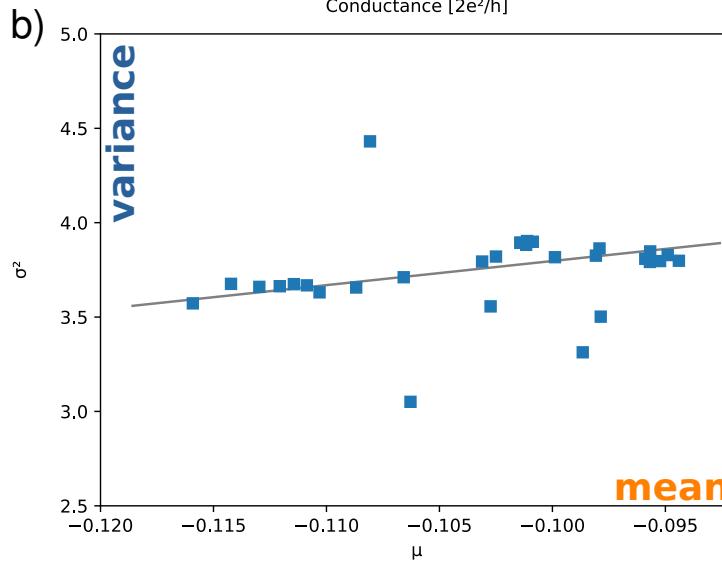
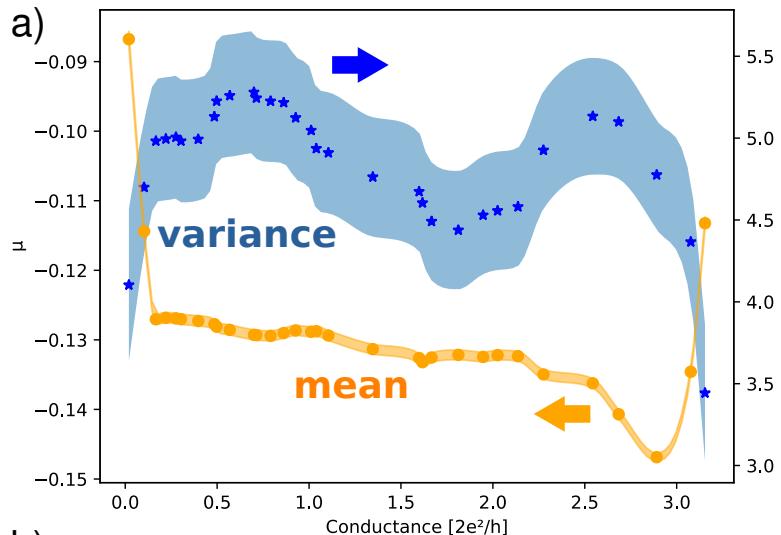
Experimental  
(expected)

Generated  
(winner)

# Potential Roughness

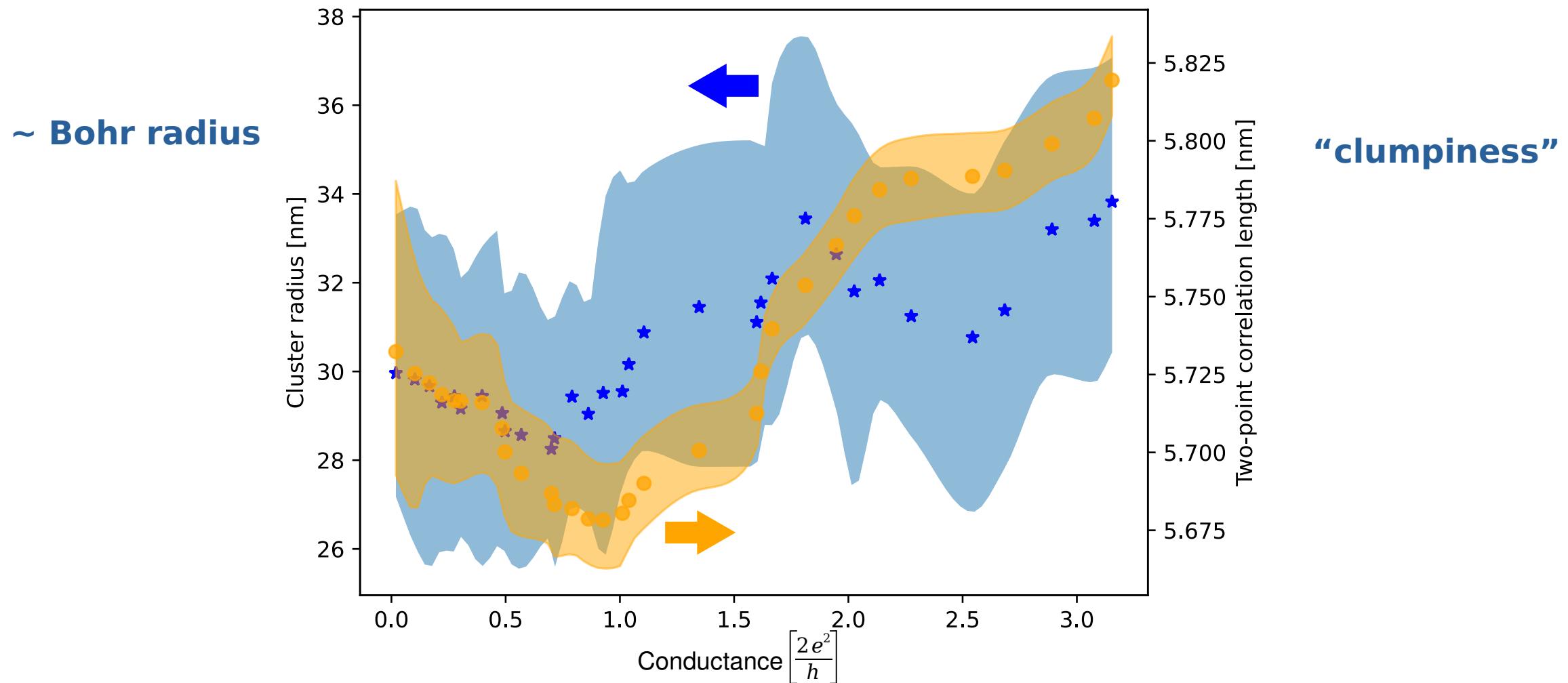


# Potential Distribution

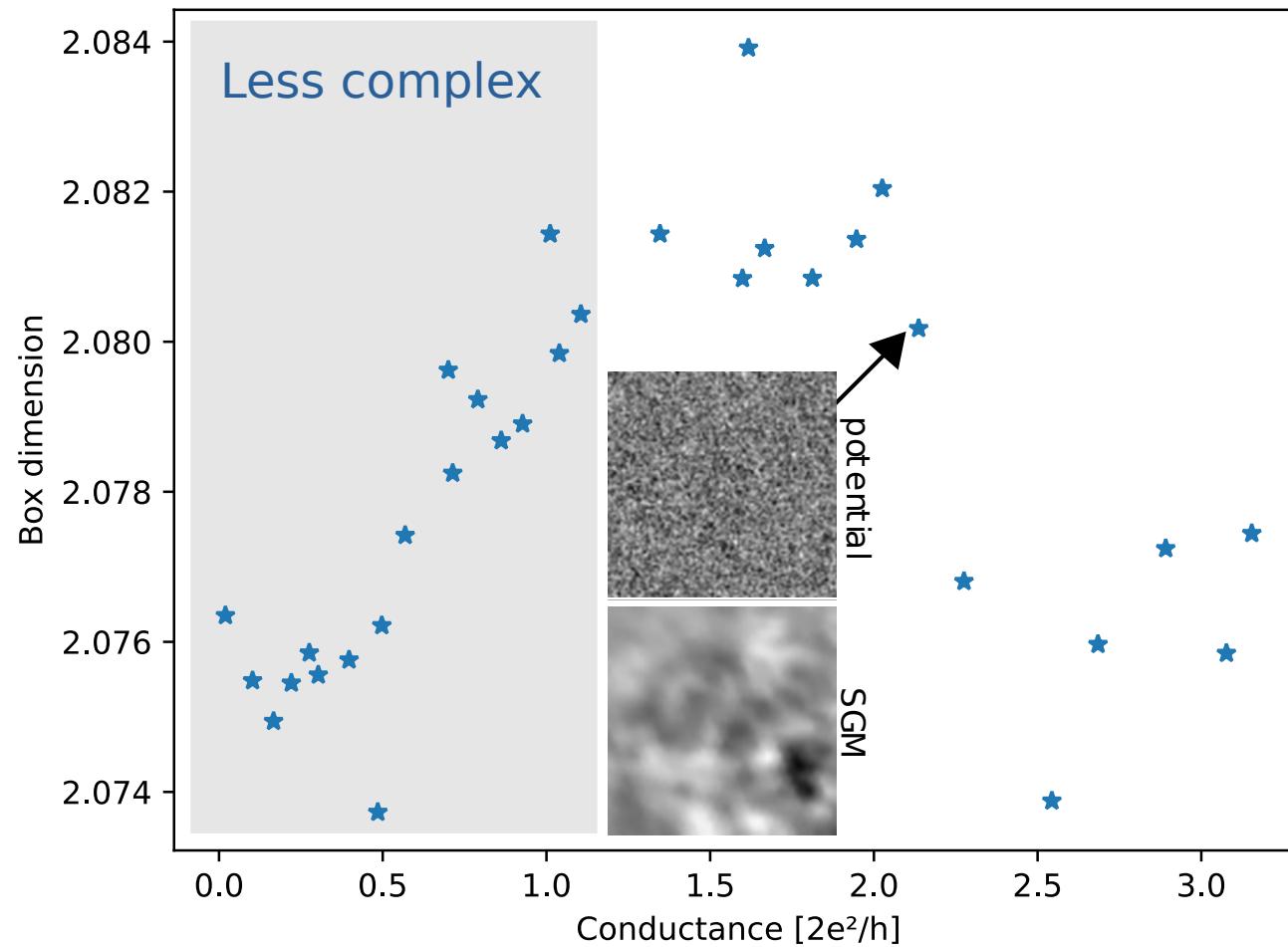


No fluctuation scaling.  
Equally important points.

# Two-Point Correlation Function

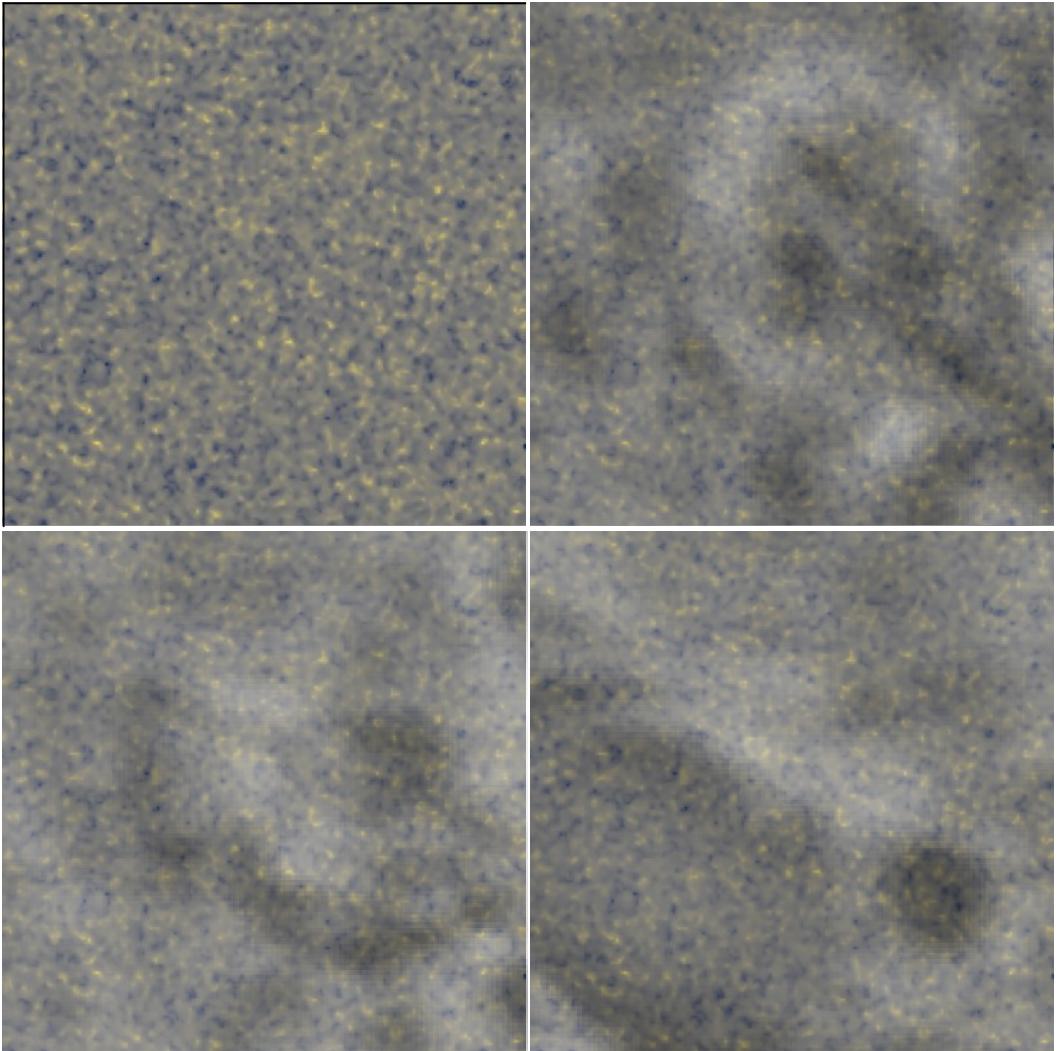


# Box Dimension



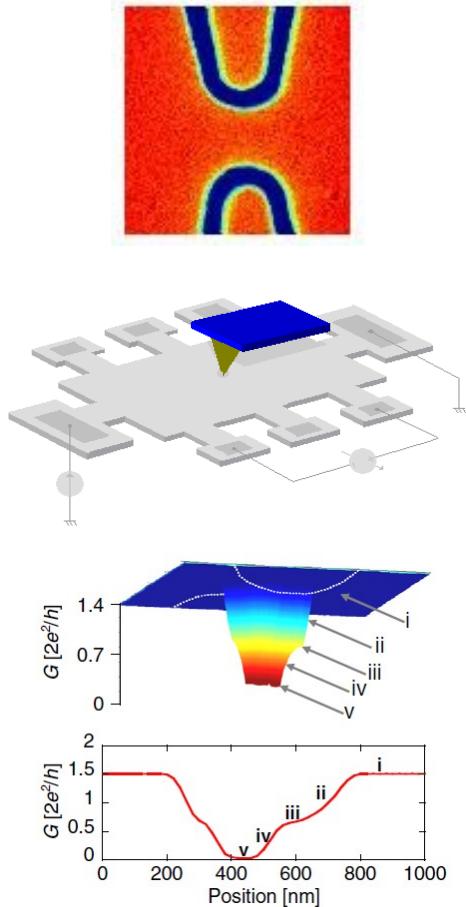
# Static Alloy Potential

$$U_{ij}^* = \frac{\langle U_{ij} \rangle}{\sigma_{ij}}$$



SGM images seem to be influenced by modes supported by the potential.

# Conclusions



## Quantum Point Contacts

- Case study: Disorder QPC
- SGM: Not simple interpretation
- Standard convolution layers not adequate
- Cellular neural networks are more adequate
- Swarming algorithm gets closer to reality (> 72 %)
- Rough potentials influence images at small base conductance
- All points in the disordered potential are equally important
- SGM images seem to be influenced by modes of the potential

## Machine learning

Useful tool for inverse problems (if properly used)  
Inverse design of new devices and materials!

# Thank You



Carlo R. daCunha

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<http://ac.nau.edu/~cc3682>



School of Informatics, Computing, and Cyber-Systems  
**Northern Arizona University**  
Flagstaff, AZ

*"Nullius addictus iurare in verba magistri, quo me cumque rapit tempestas, deferor hospes."*  
H. Flaccus