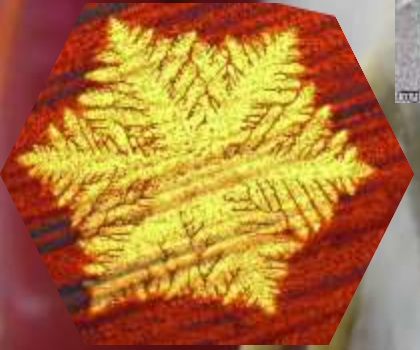
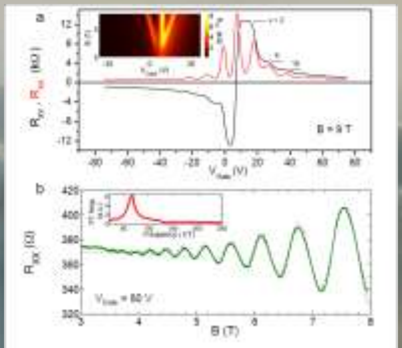
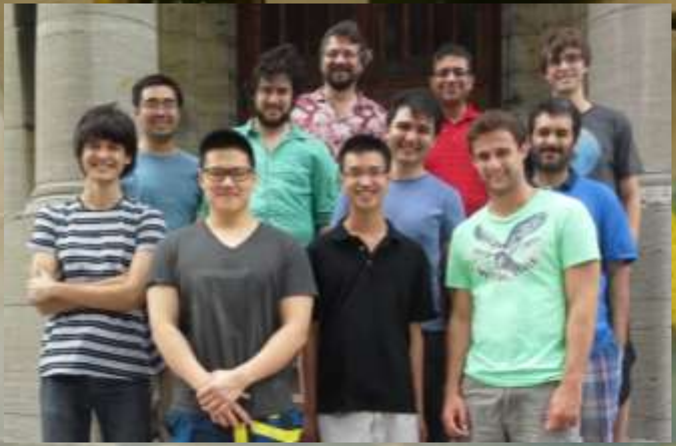
McGill

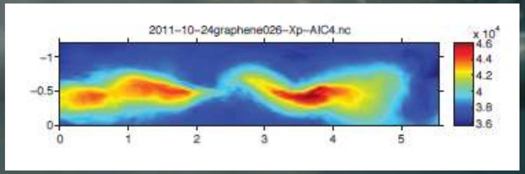
“(Quantum) Machine Learning applied to disordered systems – Daejeon

M. Hilke
(Quantum Nano Electronics Laboratory)



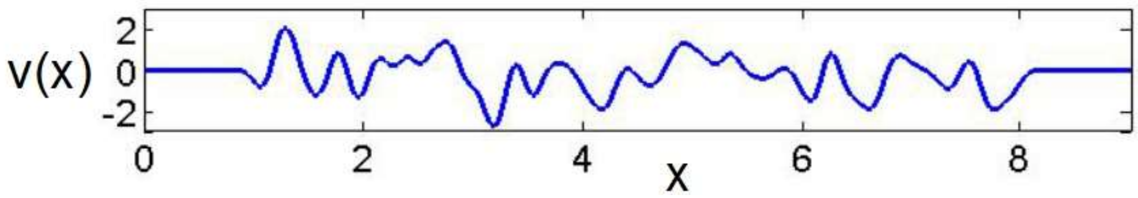




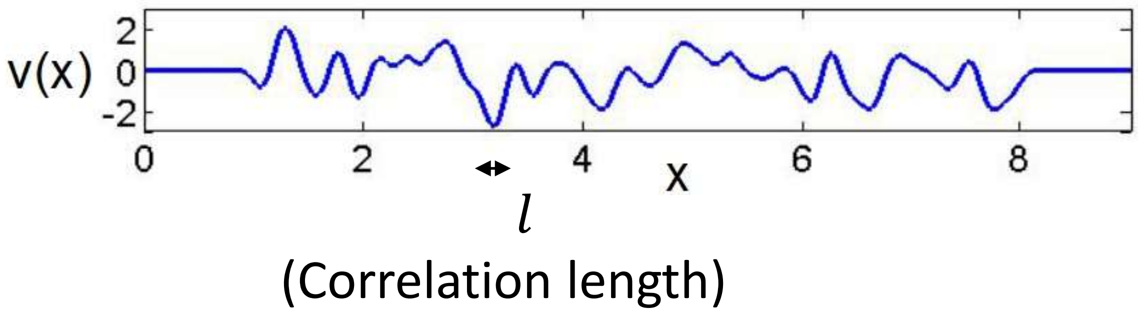


Introduction: Disorder potentials

Random potential



Random potential



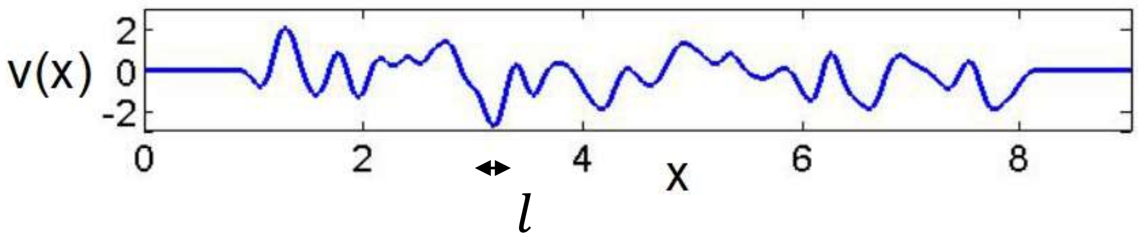
$$c_v(x) = \langle v(0)v(x)\rangle = \sigma_v^2 \mathrm{e}^{-x^2/2l^2}$$ (e.g. Gaussian)

Wave equation: $\left[\partial_x^2 + p(x)^2\right]\psi(x) = 0$

with $p(x) \equiv \partial_x P(x) = \sqrt{E - V(x)}$, $k_0 = \sqrt{E}$

Transmission $\approx e^{-\lambda x}$ → Lyapounov exponent

Random potential



(Correlation length)

$$c_v(x) = \langle v(0)v(x)\rangle = \sigma_v^2 e^{-x^2/2l^2}$$

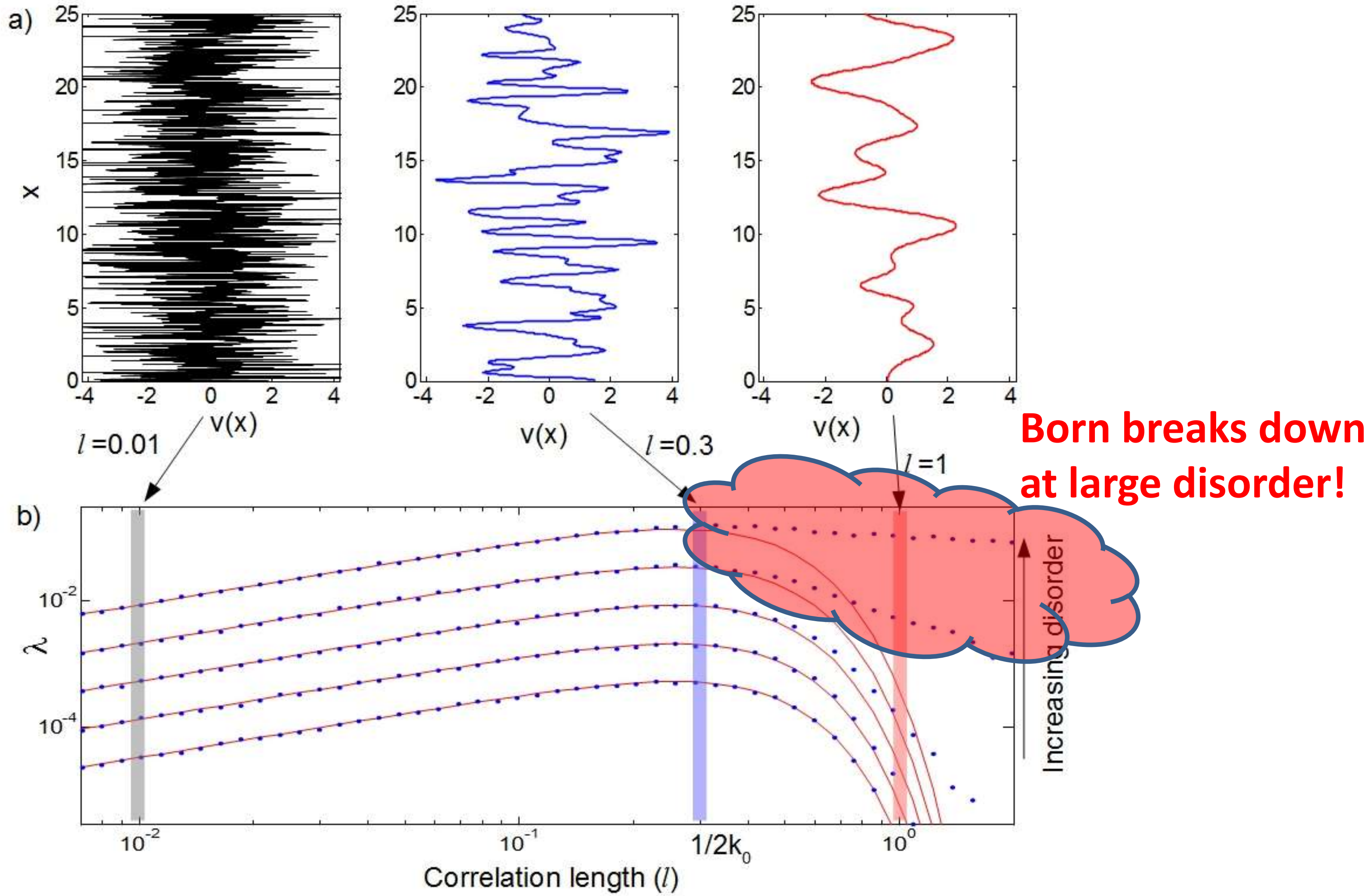
(e.g. Gaussian)

FM Izrailev, AA Krokhin, NM Makarov, Physics Reports (2011)

$$\Rightarrow \quad \lambda = \frac{\tilde{c}_v(2k_0)}{8E} = \frac{l\sigma_v^2\sqrt{2\pi}}{8E} e^{-2k_0^2 l^2}$$

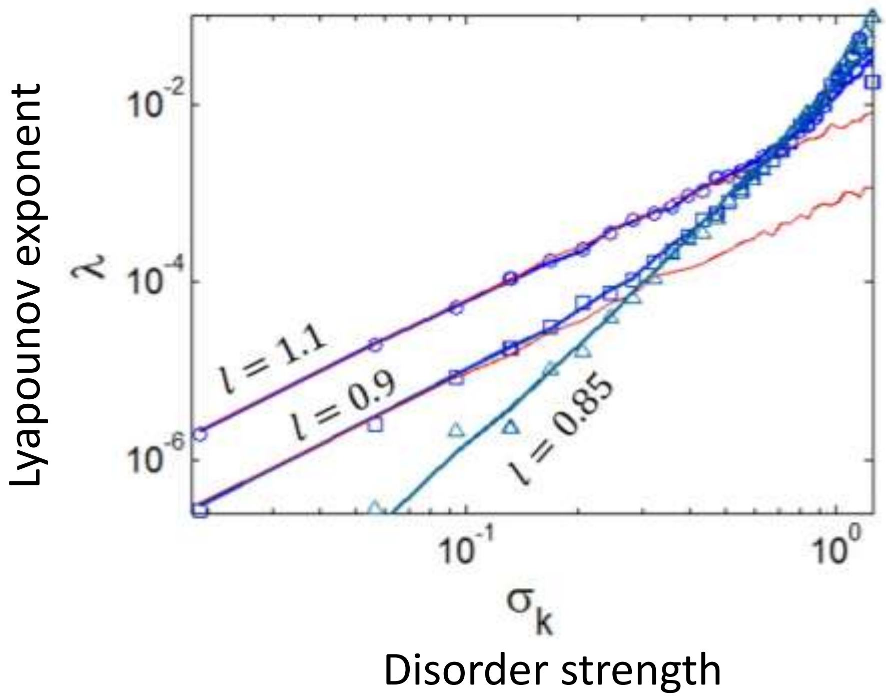
(Born approximation)

Good for weak disorder!



a)
b)
x
v(x)
l =0.01
l =0.3
l =1
λ
Increasing disorder
1/2k0
Correlation length (l)
Born breaks down
at large disorder!

Numerics and (EH)



Born approximation

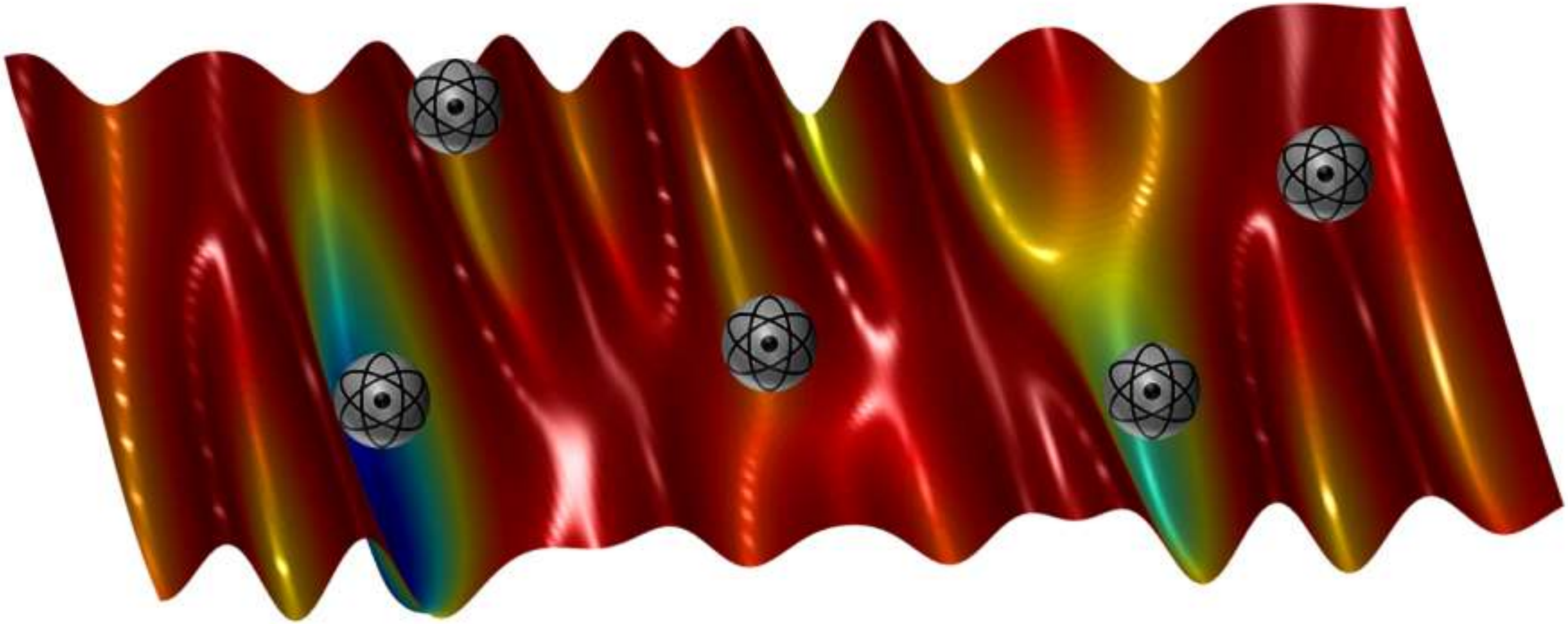
$$\lambda = \Im \int_0^\infty \mathrm{d}y \mathrm{e}^{-2\mathrm{i}k_0 y} c_p(y)$$ (EH)

$$\underbrace{\left\langle k_\nu'(x')\mathrm{e}^{-2\mathrm{i}\int_{x'}^{x} k_\nu(x'')\mathrm{d}x''} \right\rangle}_{c_p(x,x')=c_p(x-x')}$$

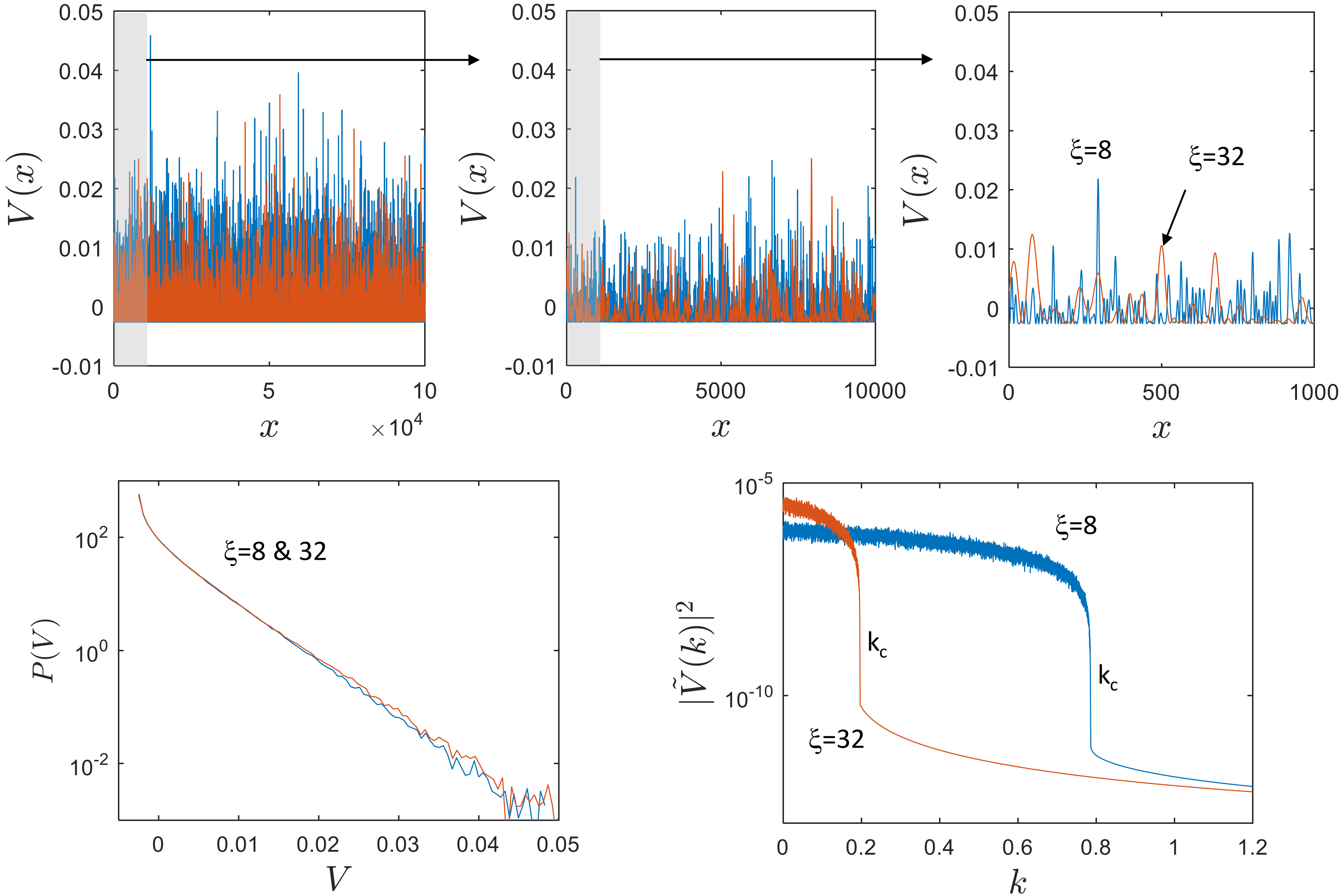
H Eleuch, M Hilke
New Journal of Physics 17 (8), 083061 (2015)

$$k_v(x) = p(x) - k_0$$

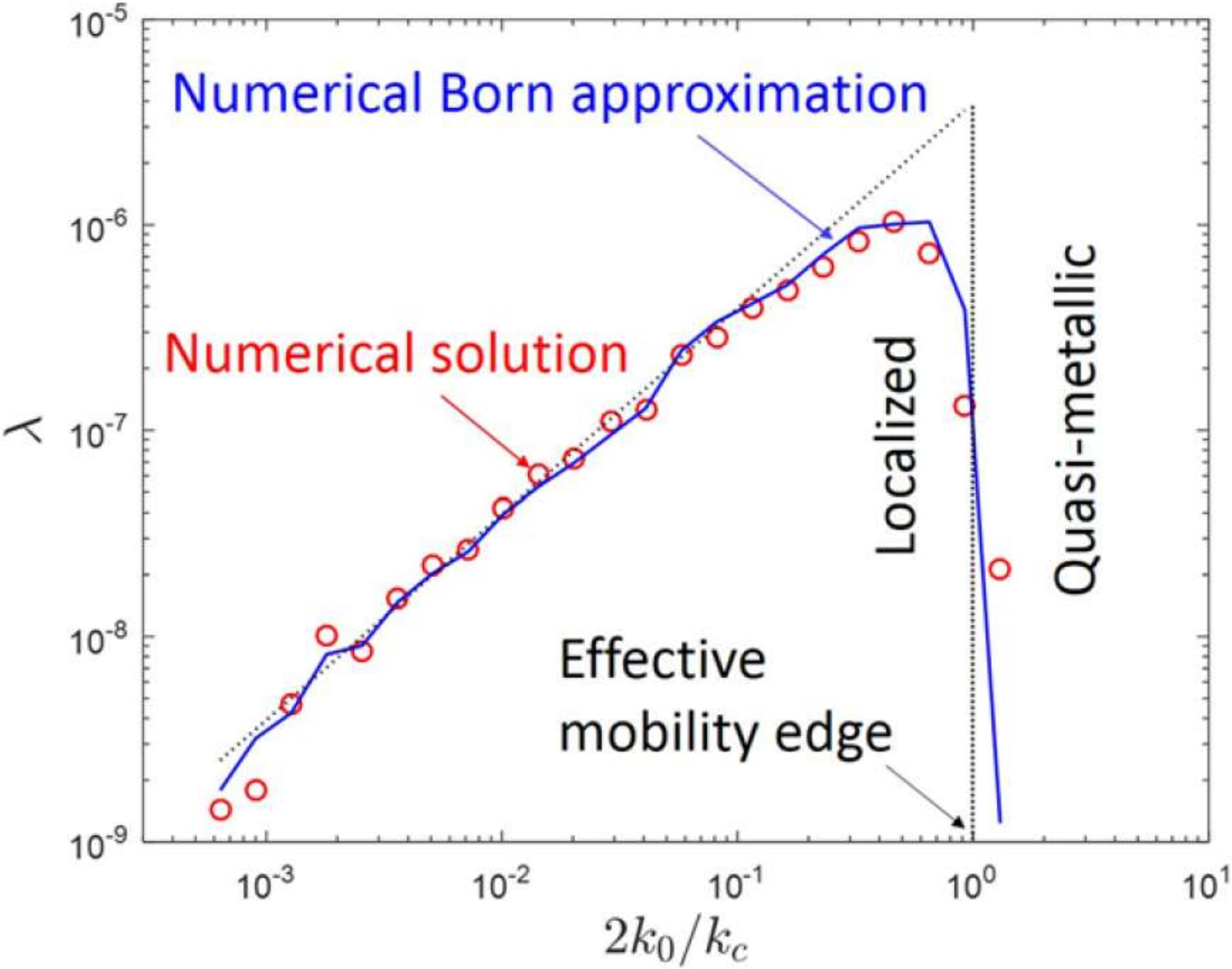
Cold atoms in a speckle potential:



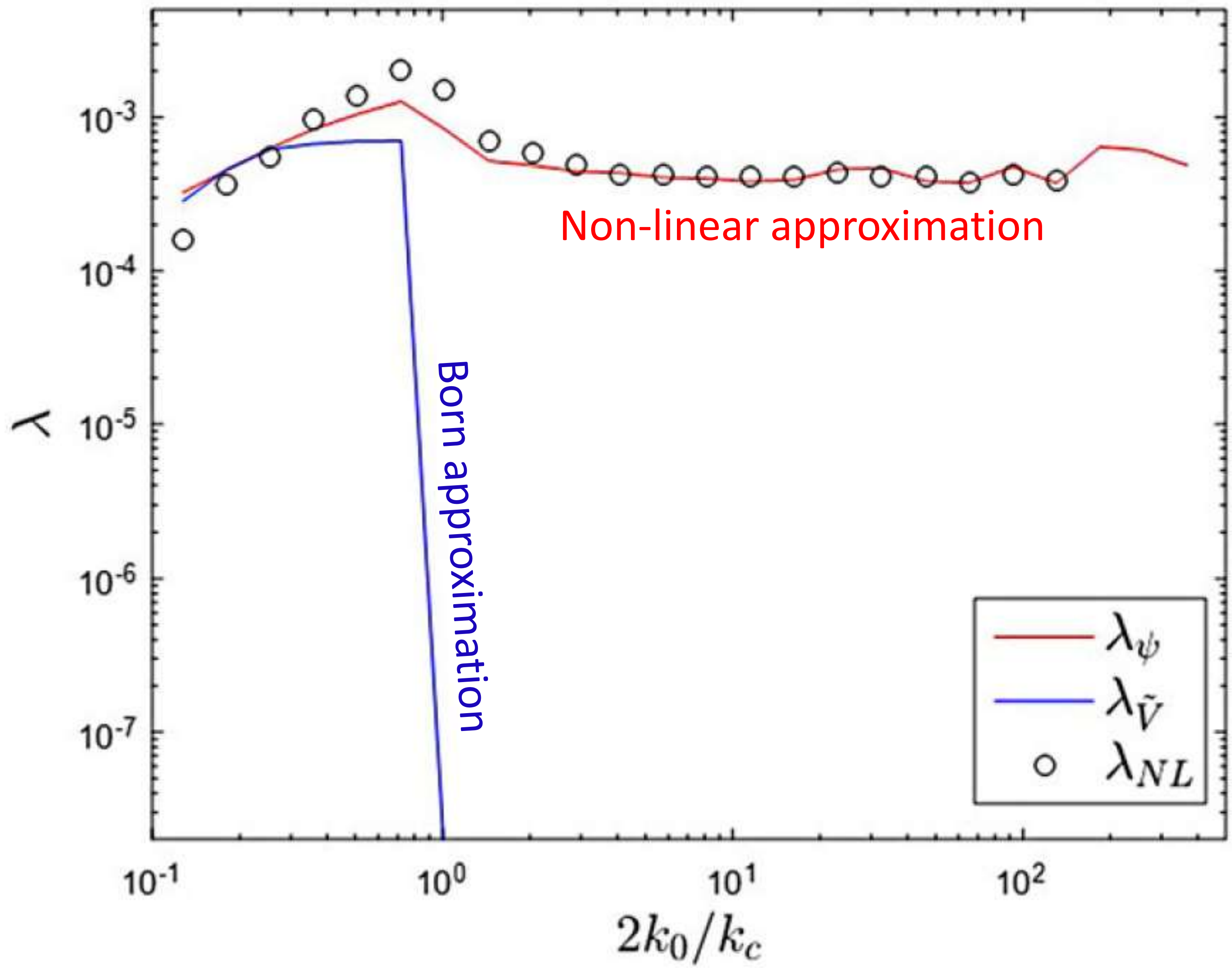
D. Clément et al., *New J. Phys.* **8**, 165 (2006).
G. Modugno, *Rep Prog. Phys.* **73**, 102401 (2010).
L. Sanchez-Palencia and M. Lewenstein, *Nat. Phys.* **6**, 87 (2010).
B. Shapiro, *J. Phys. A* **45**, 143001 (2012).
D. Delande and G. Orso, *Phys. Rev. Lett.* **113**, 060601 (2014).
L. Sanchez-Palencia et al., *Phys. Rev. Lett.* **98**, 210401 (2007).
J. Billy et al., *Nature* **453**, 891 (2008).
M. Piraud and L. Sanchez-Palencia, *EPJ* **217**, 91 (2013).



Fourier transform: band edge

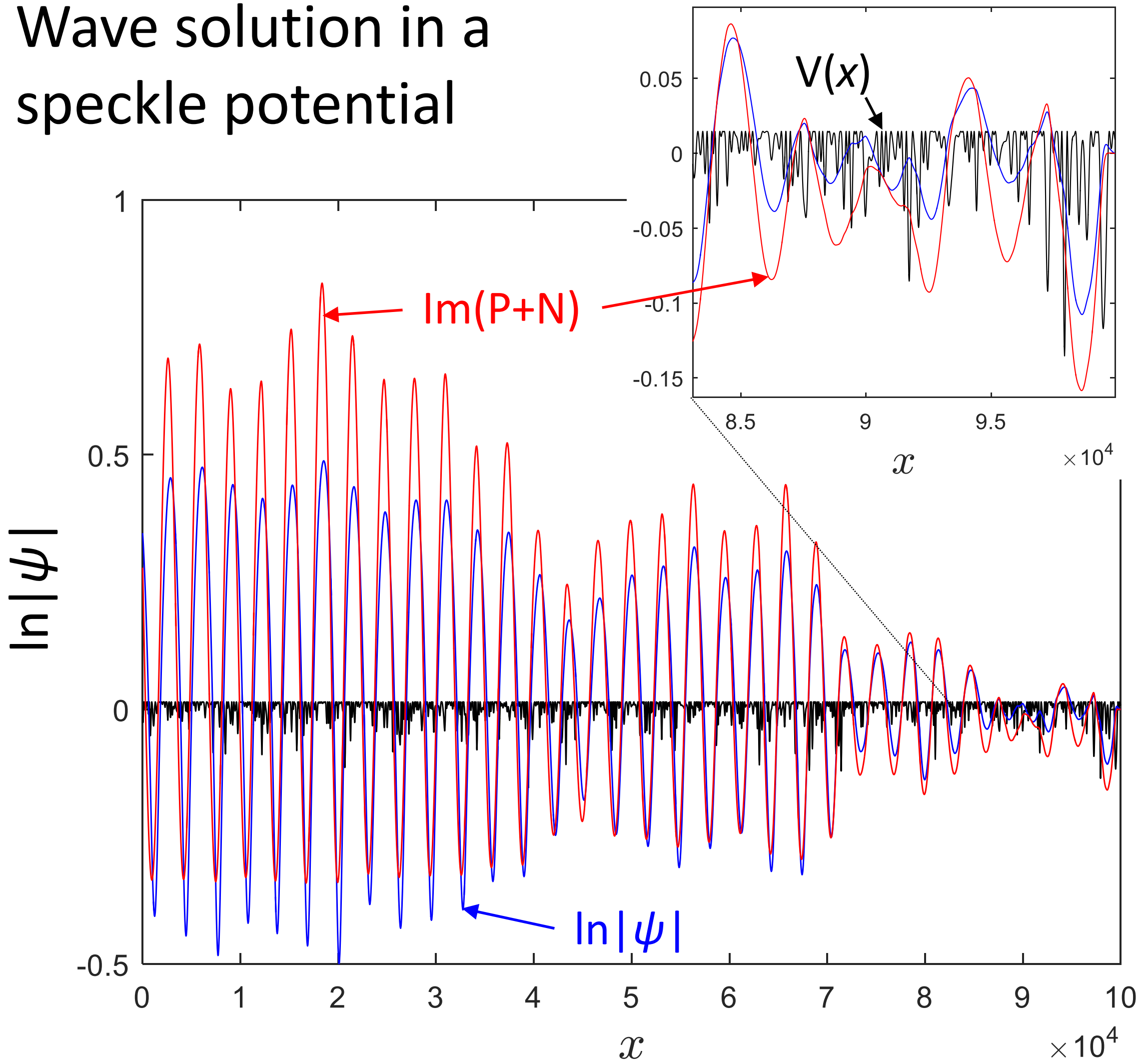


weak disorder



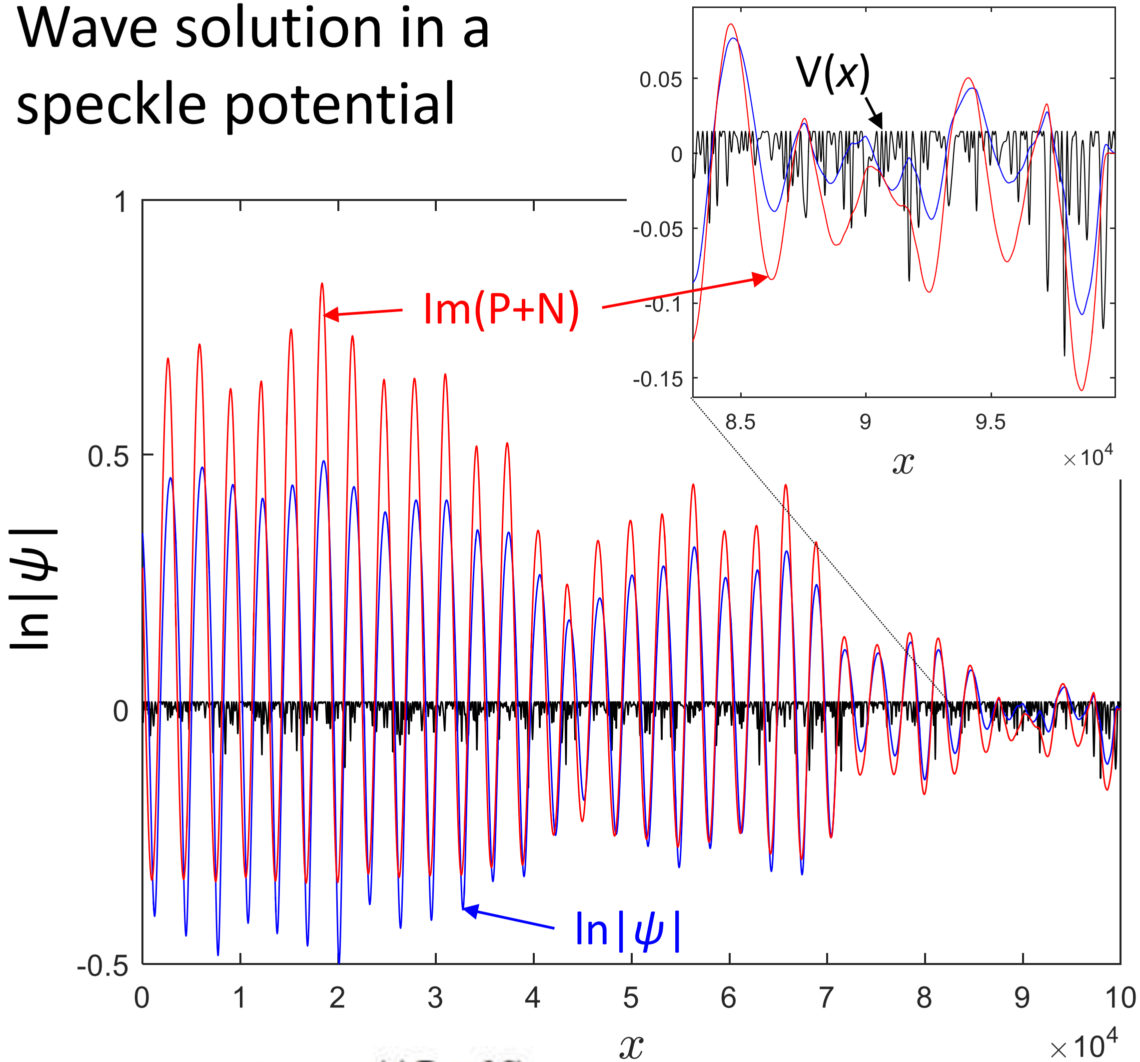
strong disorder

Wave solution in a speckle potential



weak potential

Wave solution in a speckle potential



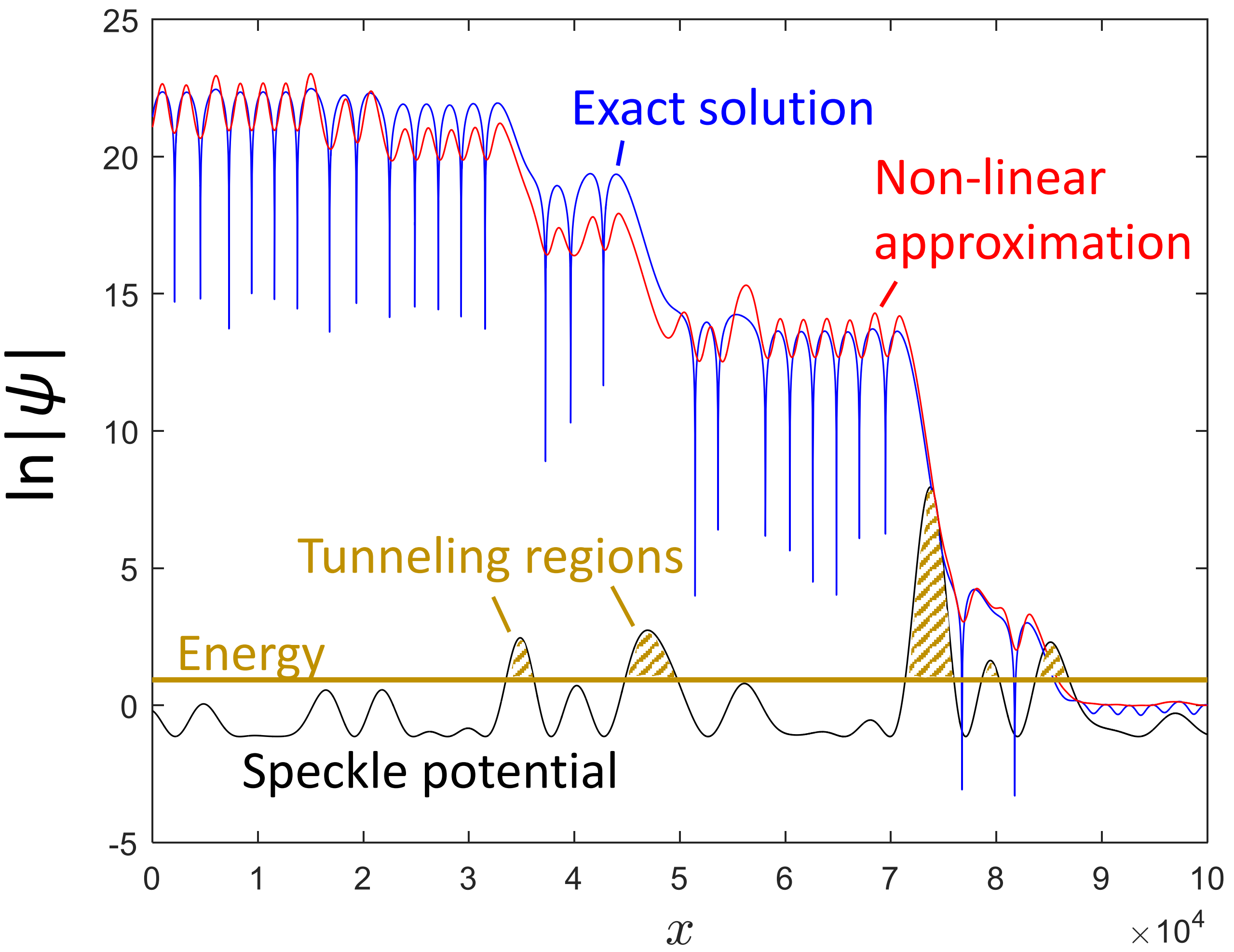
$$\psi(x) = e^{i(P+N)}$$

$$\partial_x N(x) = -e^{-2i\,P(x)} \int^x e^{2i\,P(x')}\,p'(x')\,dx'$$

non-linear approximation

weak potential

Can you obtain V(r) from |ψ| ?



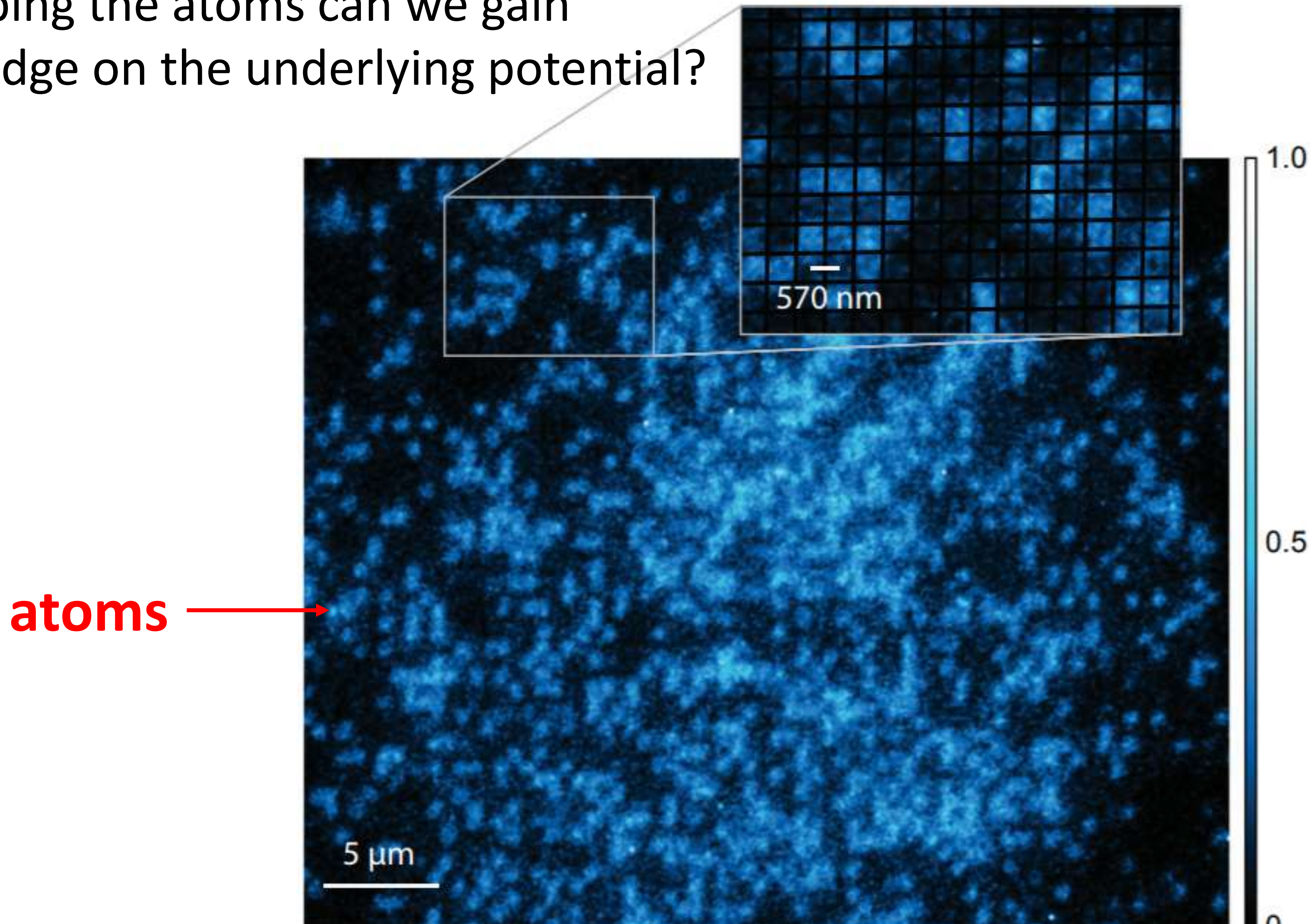
strong potential

M. Hilke and H. Eleuch, *Ann. Phys.* (*Berlin*) **2017**, 1600347

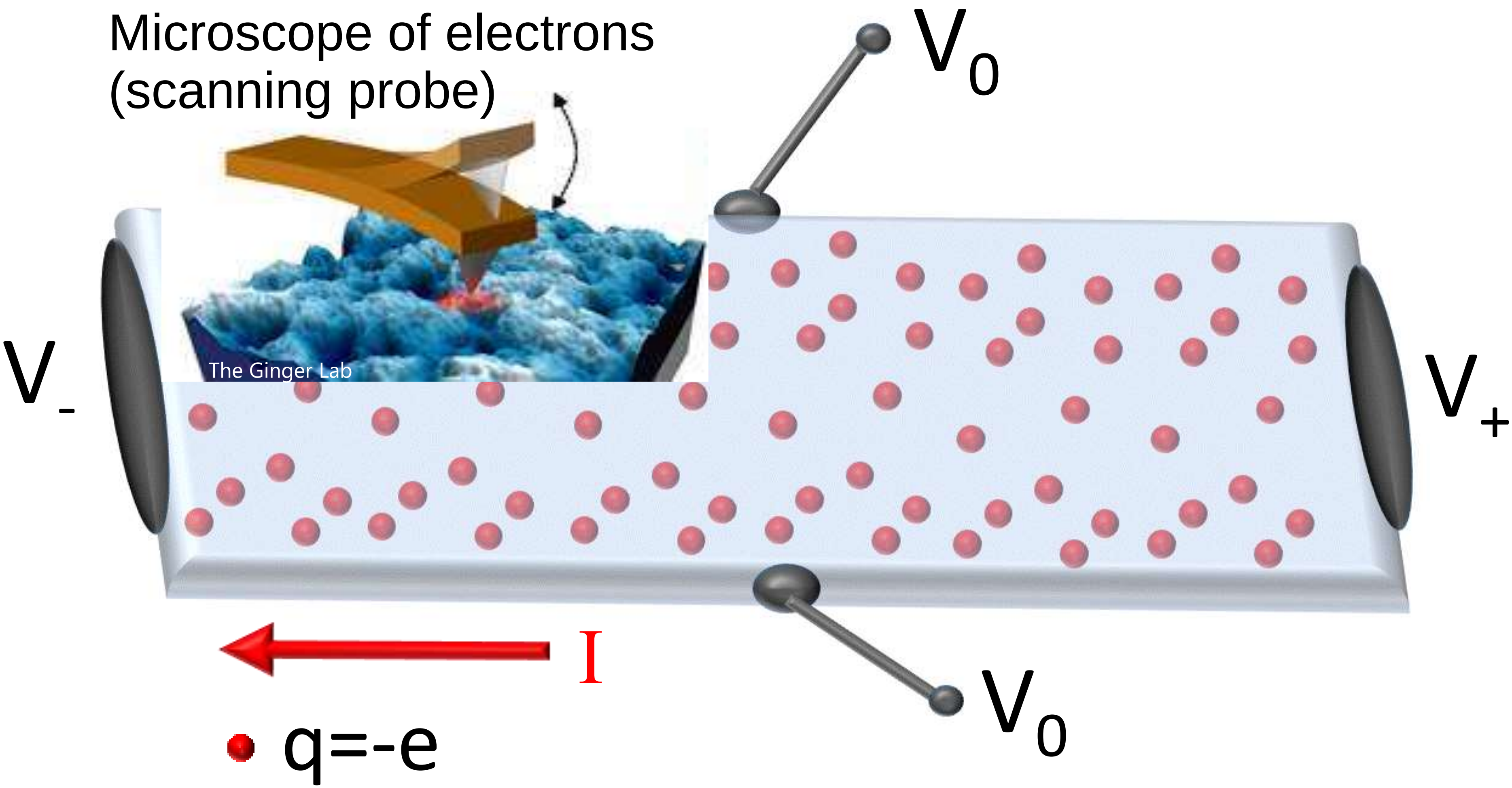
What is the underlying potential?

2D

By probing the atoms can we gain knowledge on the underlying potential?

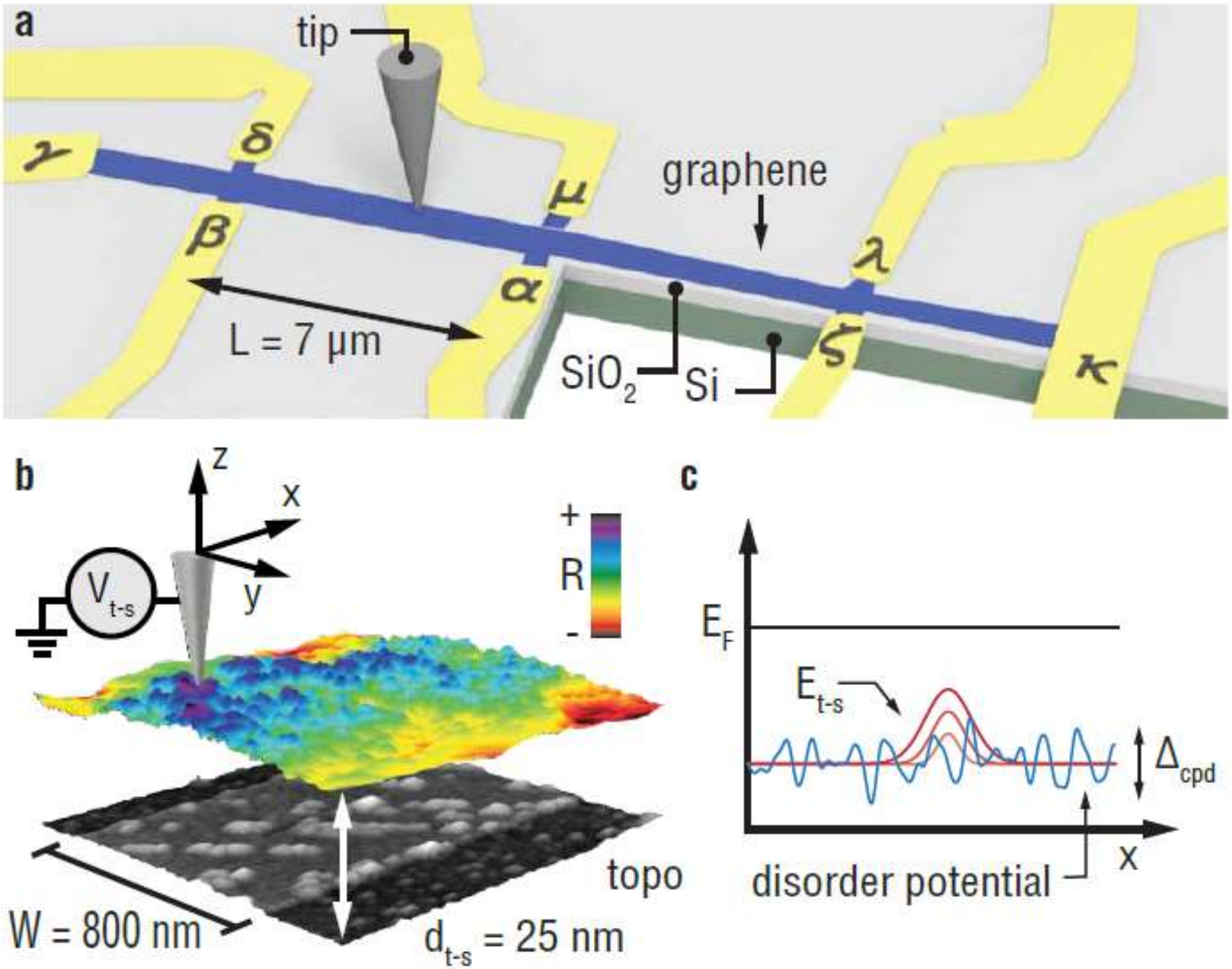


Li atoms trapped in an effective 2D potential (Greiner group)



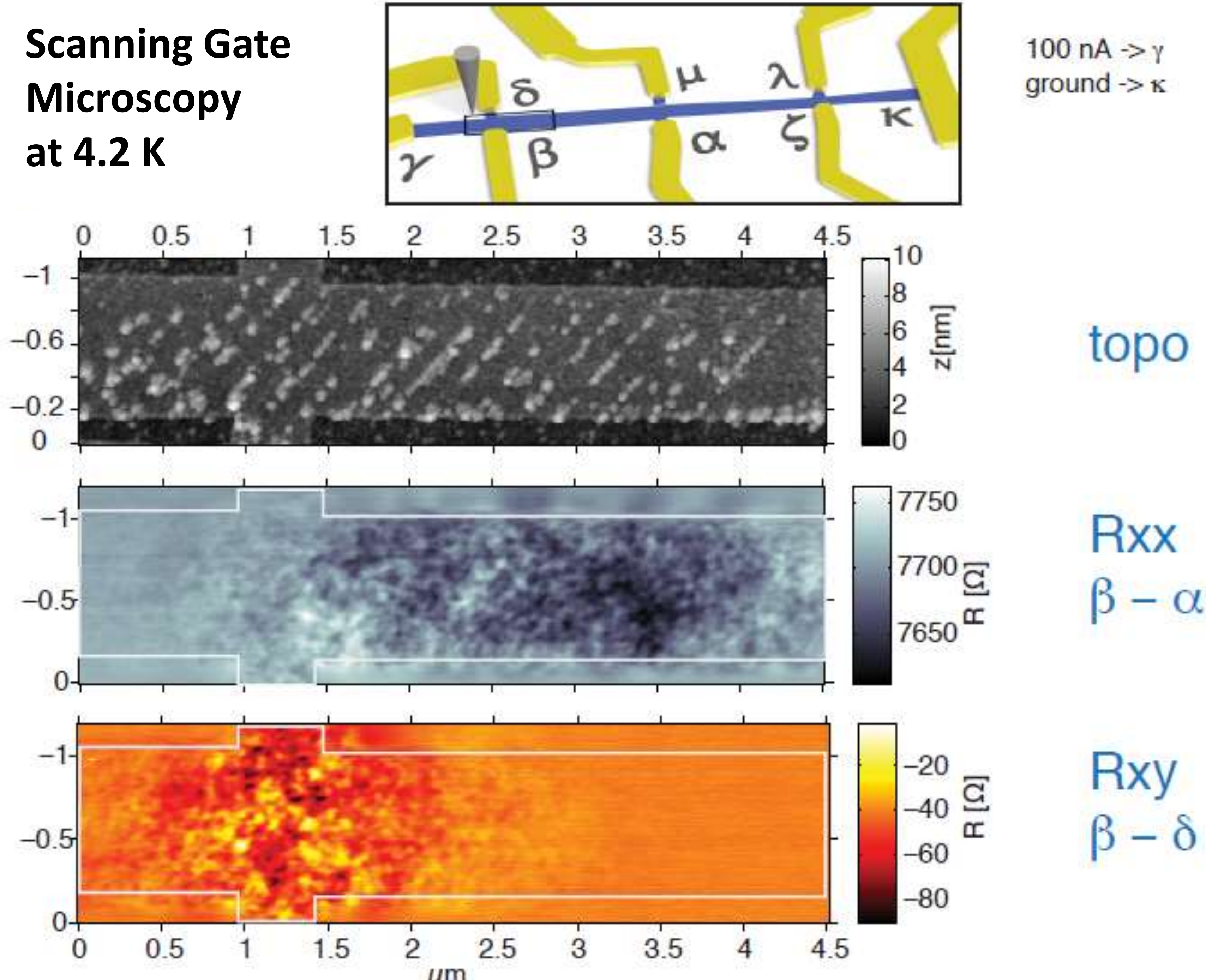
Flow of electrons through a disordered conductor

Scanning gate with a low temperature AFM

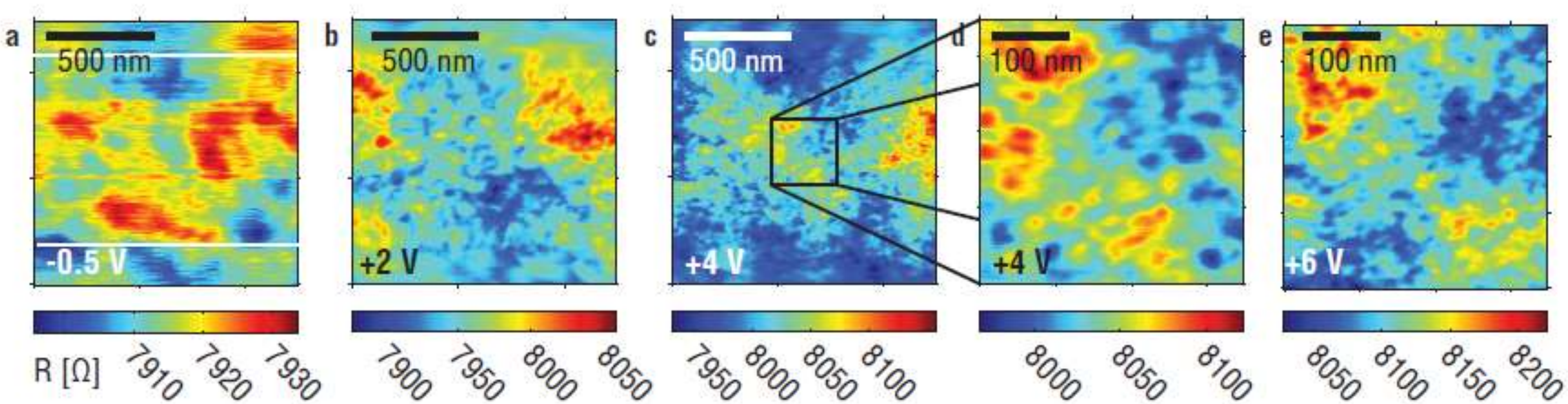


With J. Hedberg and J. Renard et al (2013)

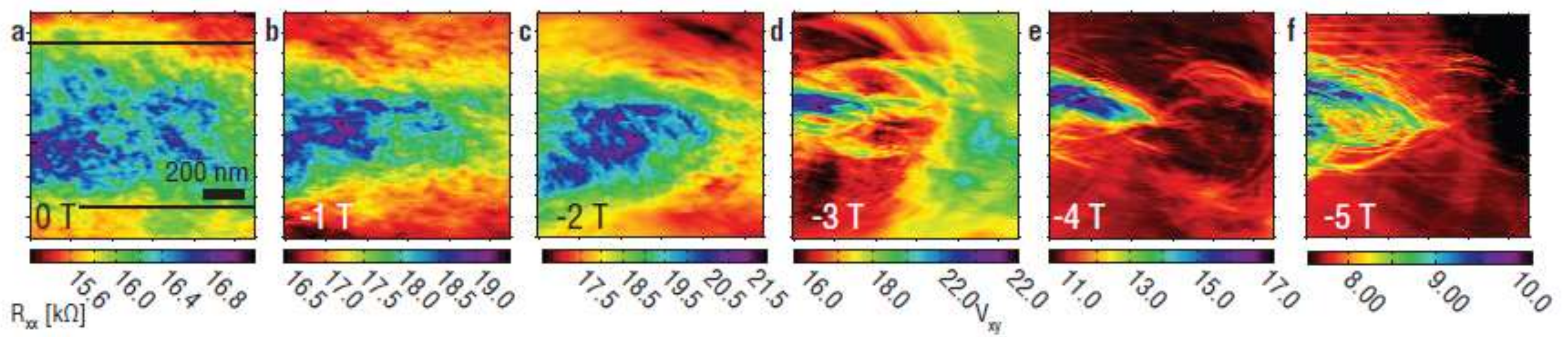
Scanning Gate Microscopy at 4.2 K



Increasing AFM tip – sample bias



Increasing magnetic field



fluctuations → “circles”

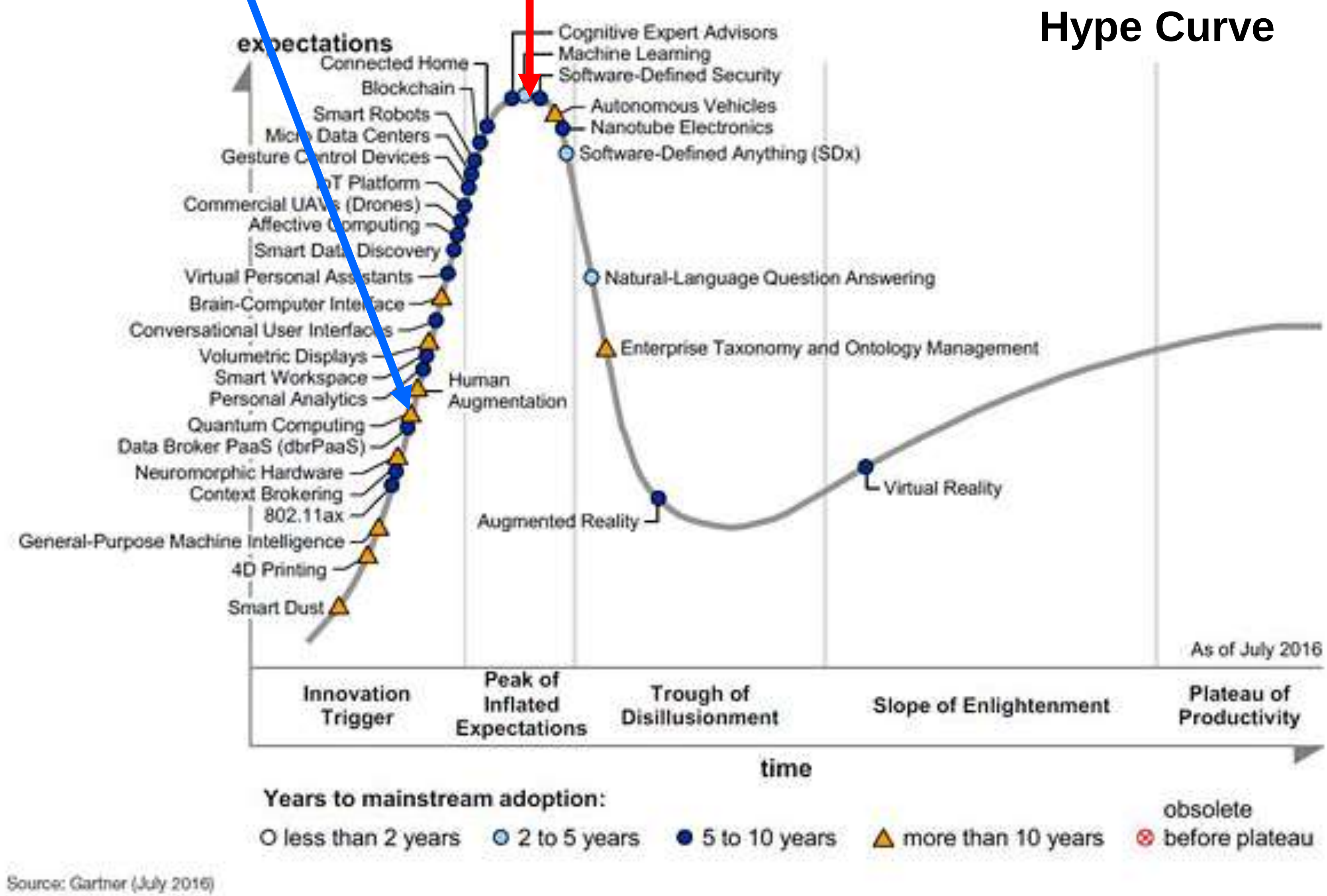
What is the underlying disorder potential?

End of introduction

Montreal, emerging as AI's world center

Montreal is a true melting pot for Artificial Intelligence. The meeting between several attractive AI poles creates excitement in Montreal.

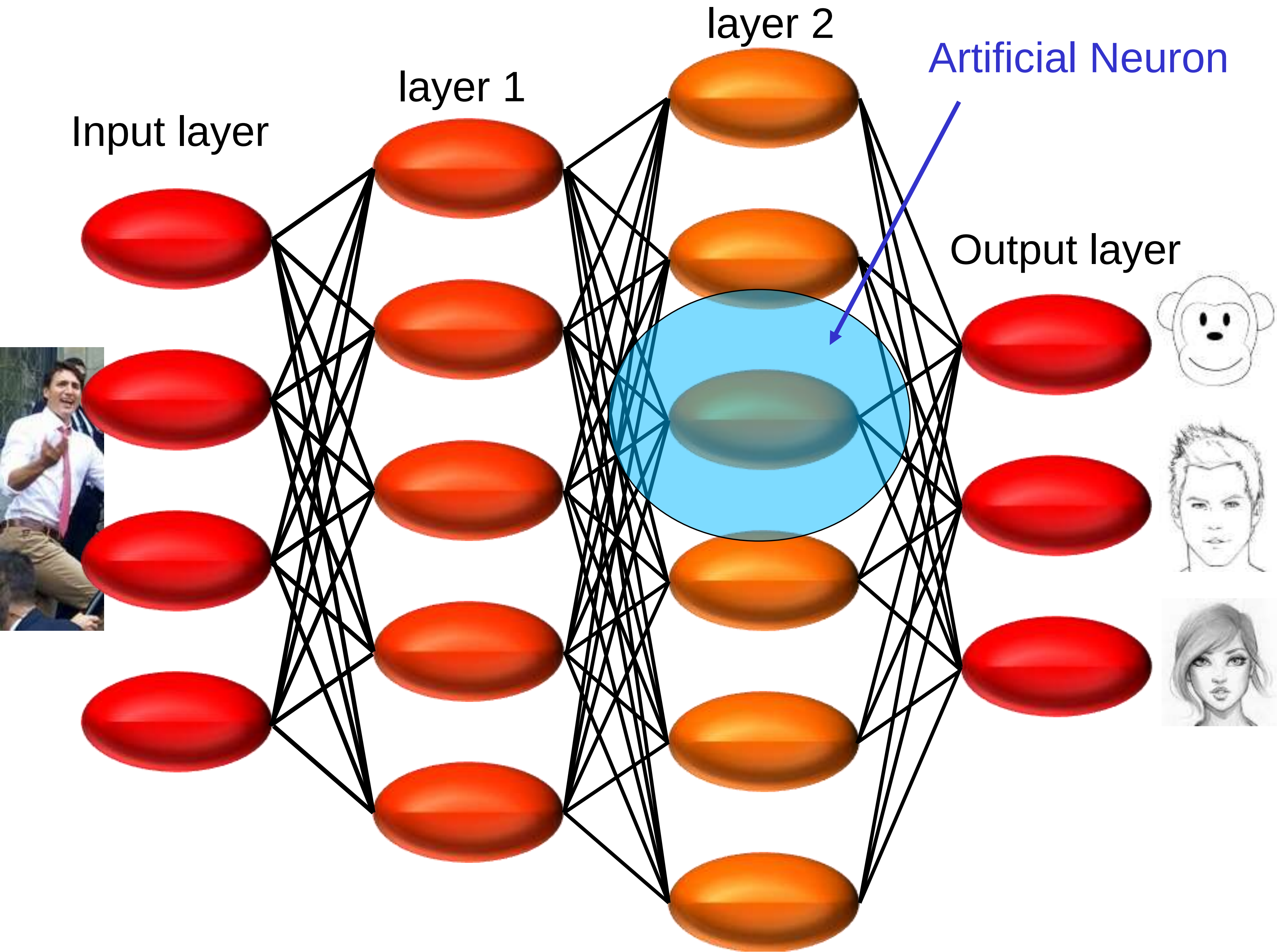
Quantum Machine Learning?



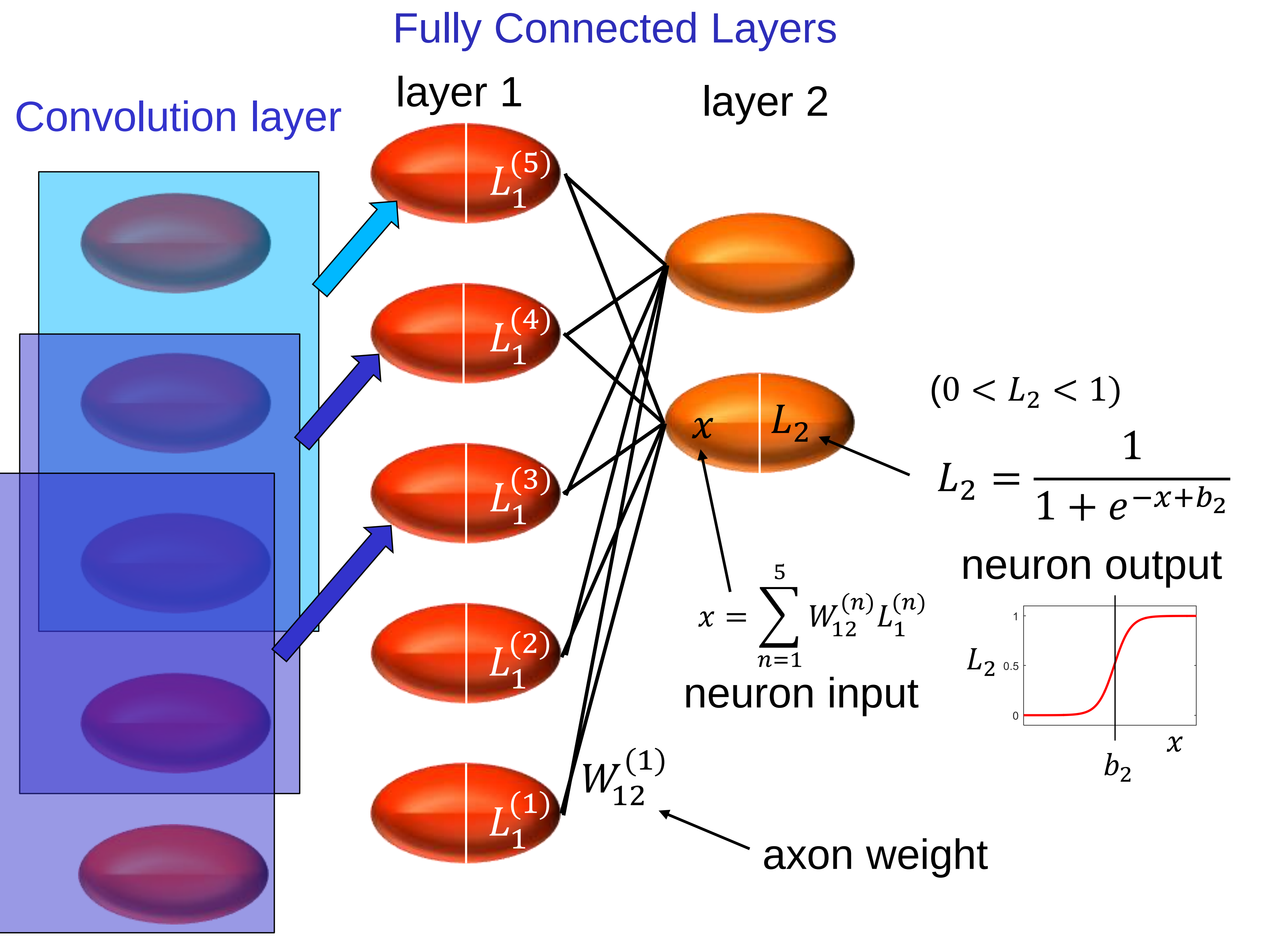
Machine Learning:

With David Ittah, An Vuong, Dominic Bernardi, Andre Cheng, Diego Lopez

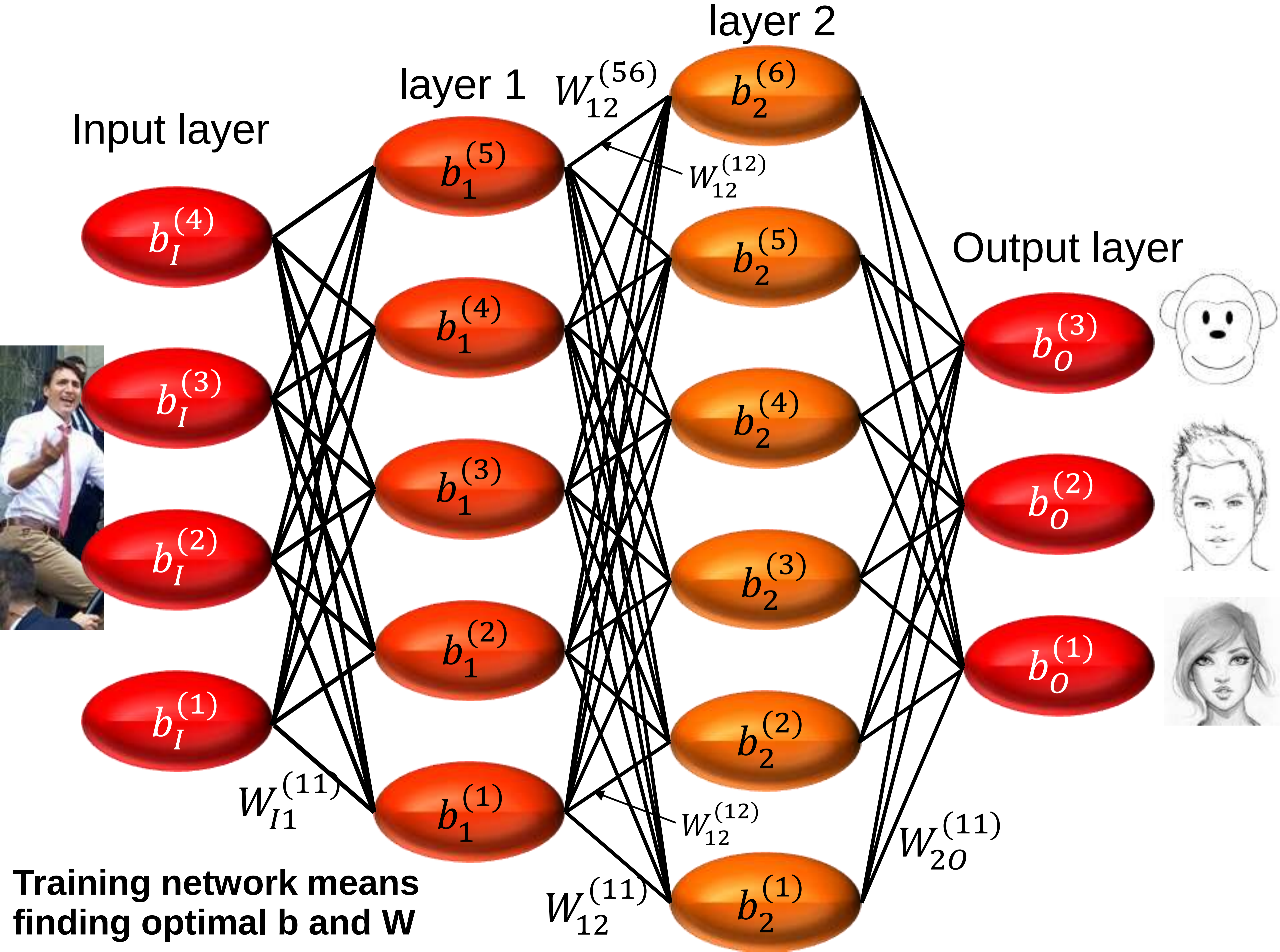
Principle of Deep Convolution Neural Network for Face Recognition



layer 2
Artificial Neuron
layer 1
Input layer
Output layer



Fully Connected Layers
Convolution layer
layer 1
layer 2
$L_1^{(5)}$
$L_1^{(4)}$
$L_1^{(3)}$
$L_1^{(2)}$
$L_1^{(1)}$
x
L_2
$(0 < L_2 < 1)$
$L_2 = \frac{1}{1 + e^{-x+b_2}}$
neuron output
$x = \sum_{n=1}^{5} W_{12}^{(n)} L_1^{(n)}$
neuron input
$W_{12}^{(1)}$
axon weight
L_2
1
0.5
0
b_2
x



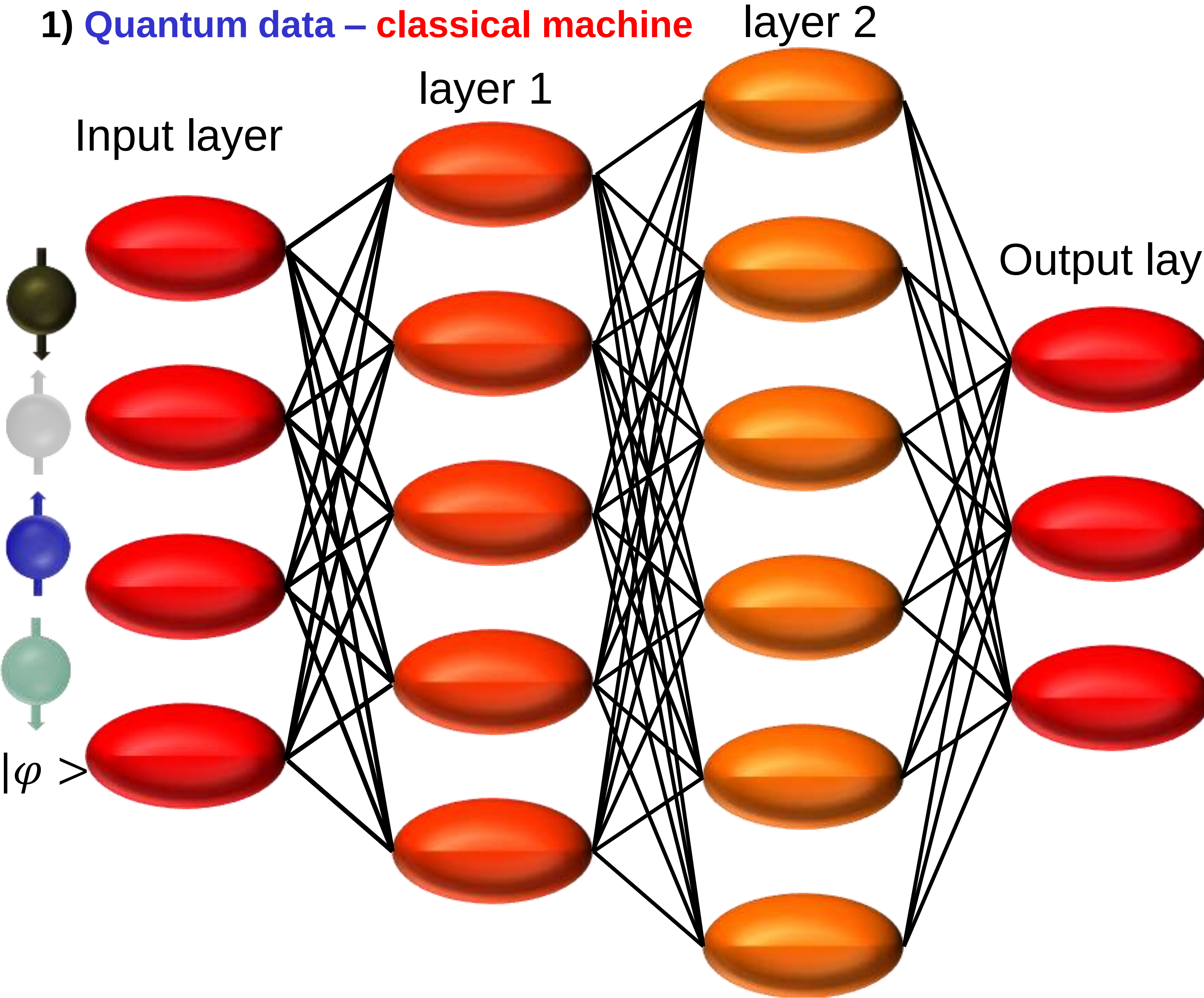
Training network means finding optimal b and W

That was Classical Machine Learning

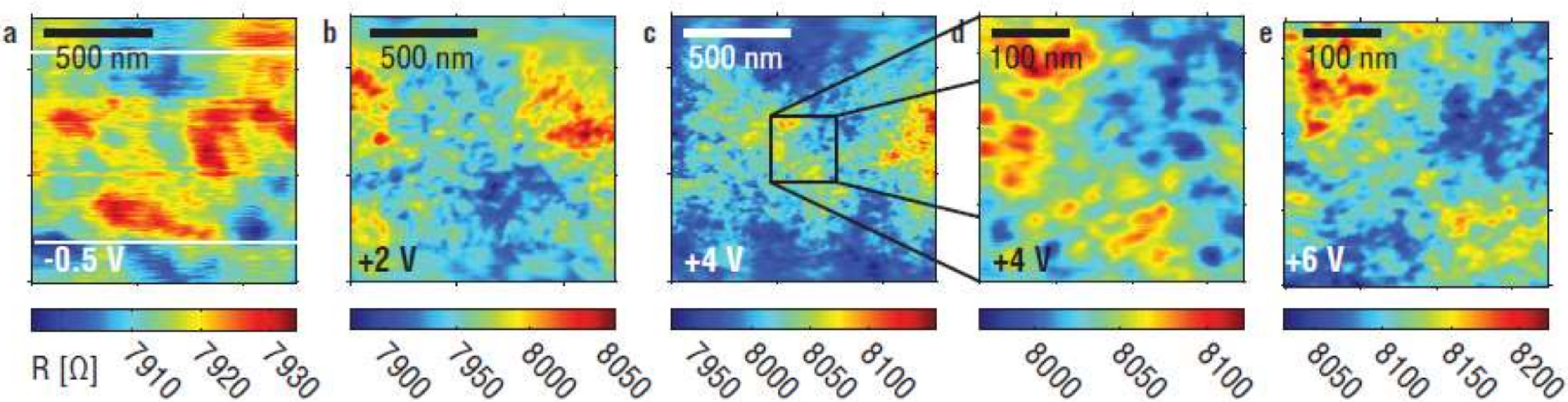
Quantum Machine Learning (3 categories)

1) Quantum data – classical machine
2) Classical data – quantum machine
3) Quantum data – quantum machine

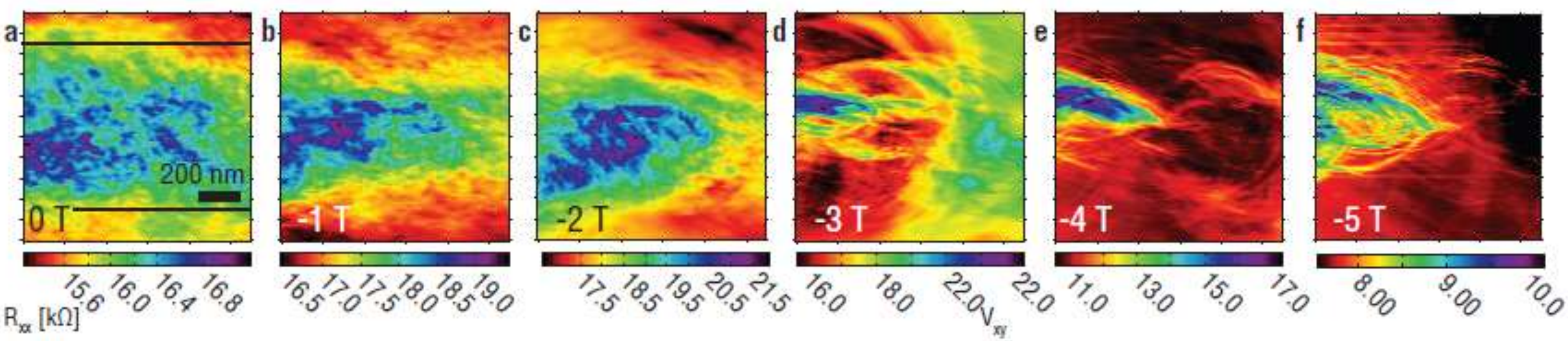
1) Quantum data – classical machine



Increasing AFM tip – sample bias

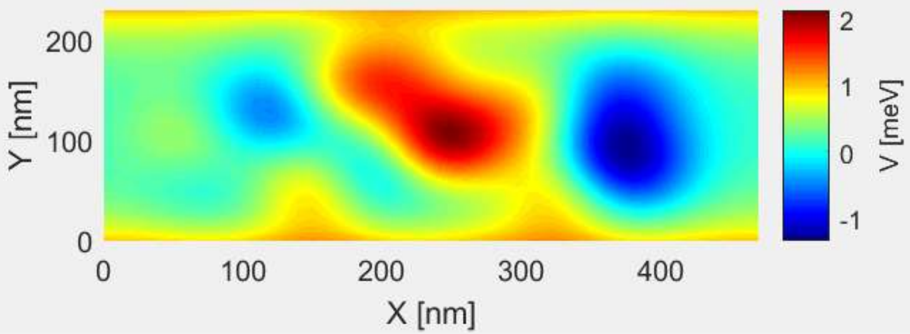


Increasing magnetic field

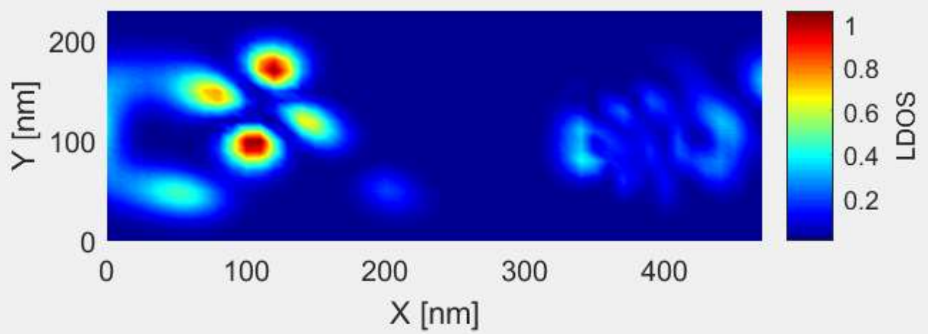


fluctuations → “circles”

What is the underlying disorder potential?



Disorder potential

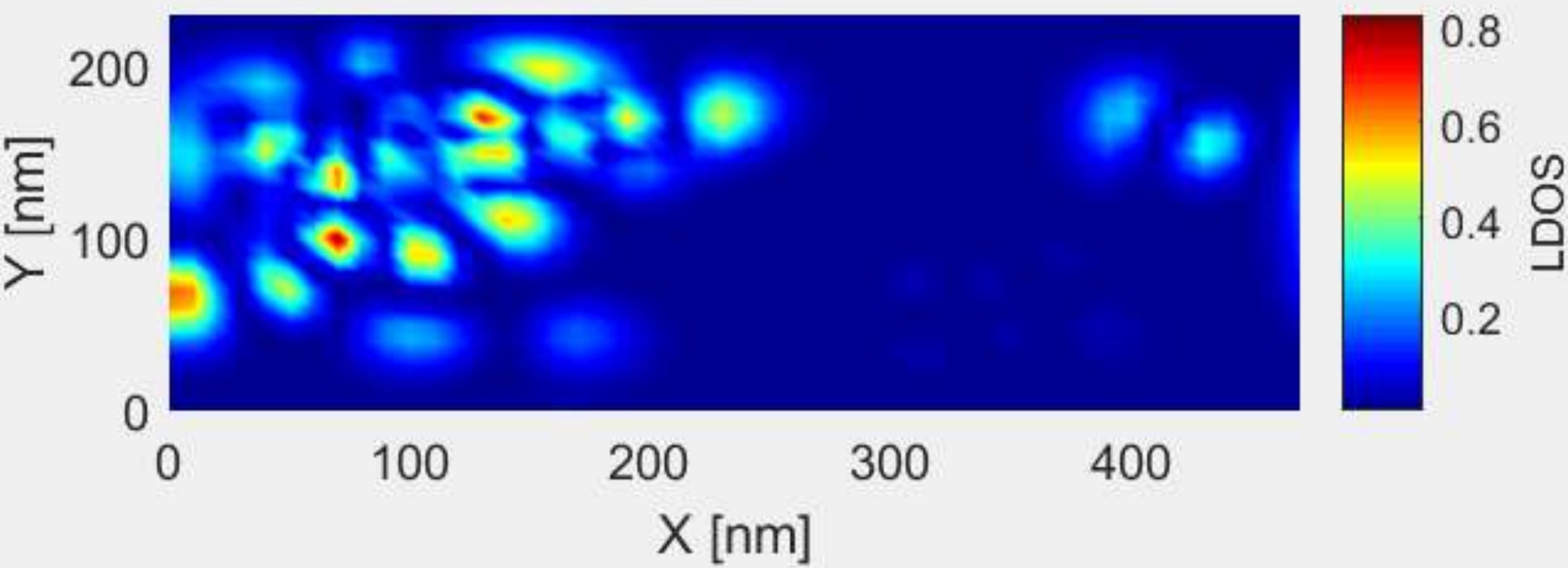


Electron density

Quantum Calculation (solving Schrödinger equation) and computing the Local Density of State at E_0

This is the electron density, what is the corresponding potential?

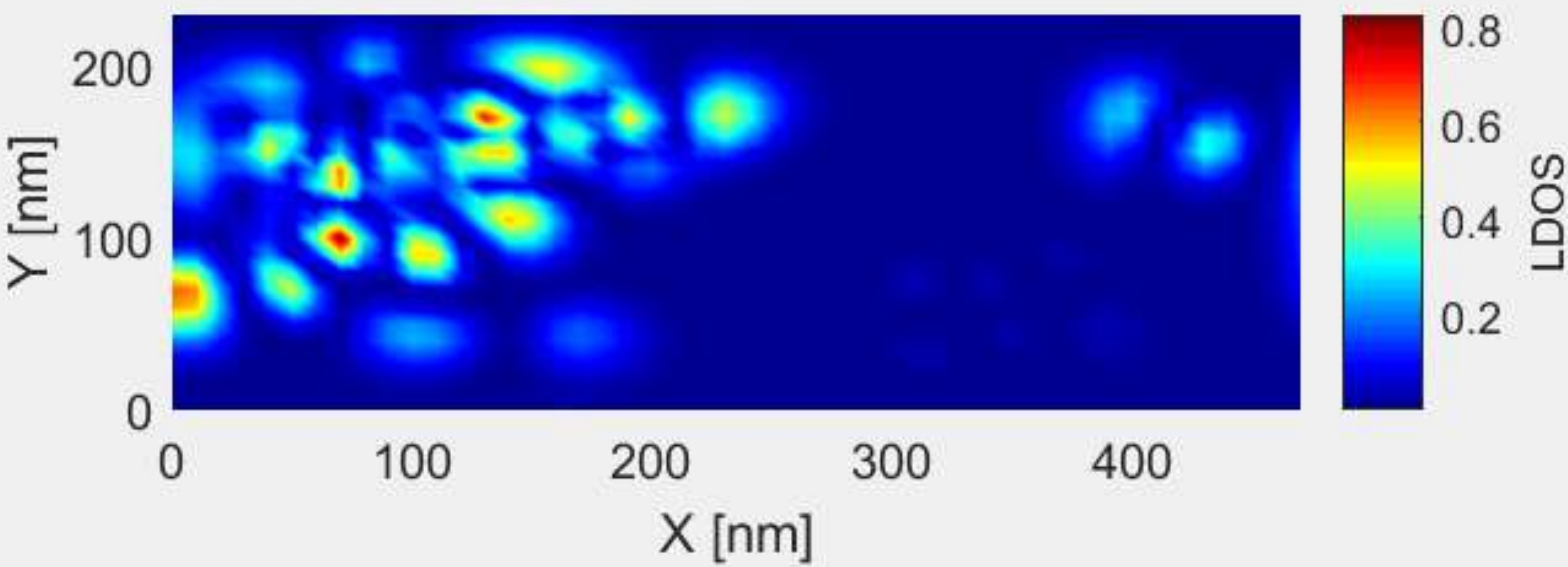
=> Hard problem

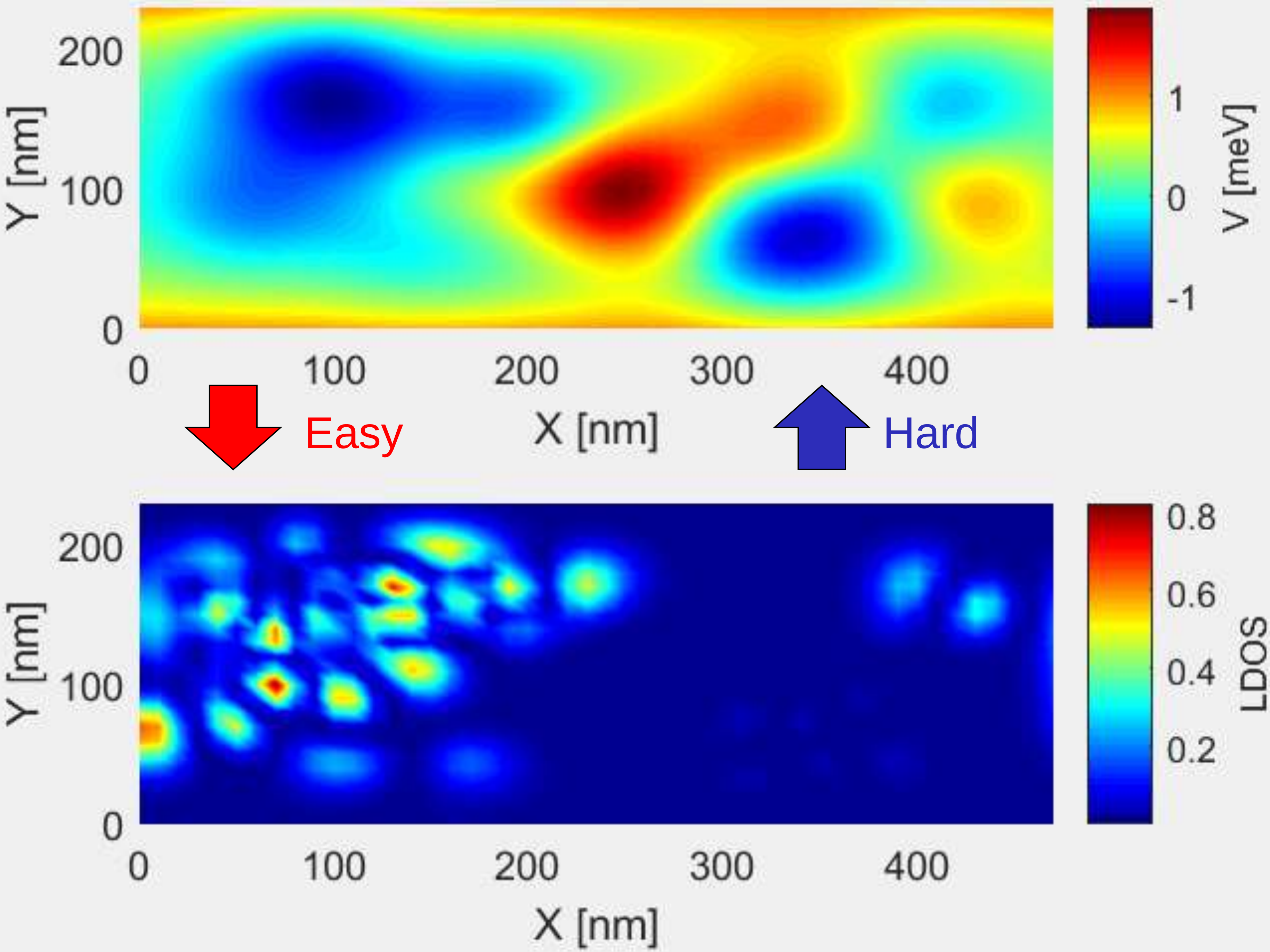


This is the electron density, what is the corresponding potential?

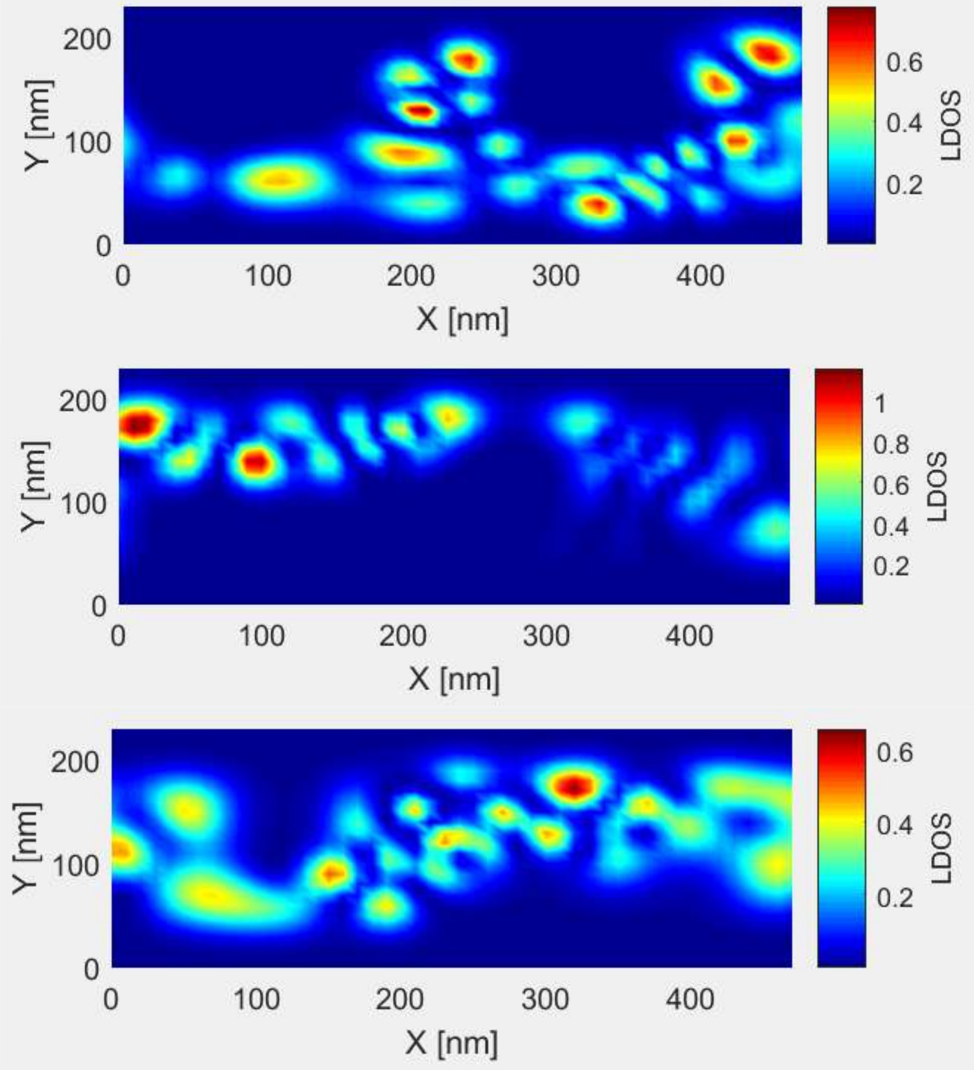
=> Hard problem

Can Quantum Machine Learning help?

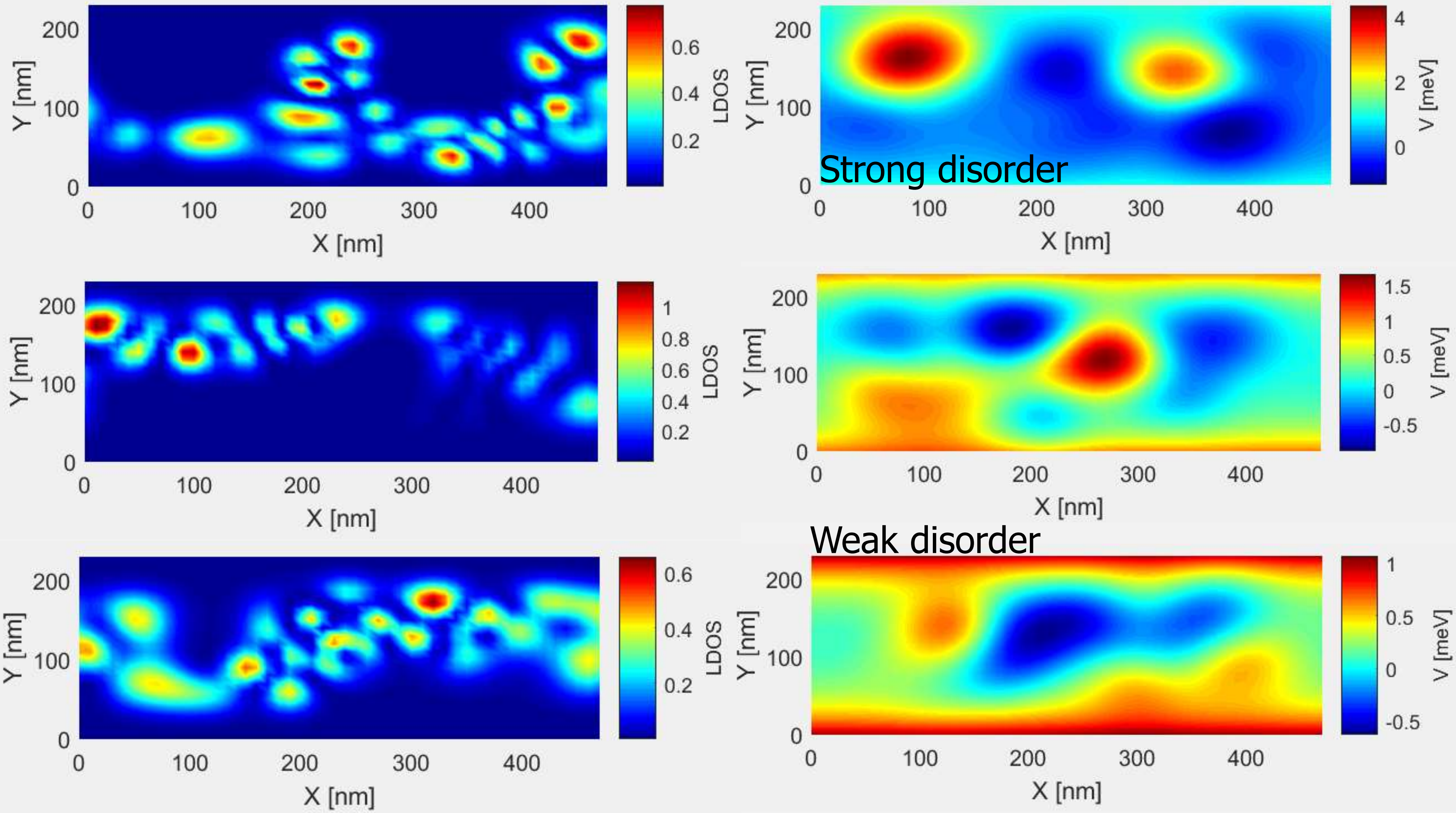




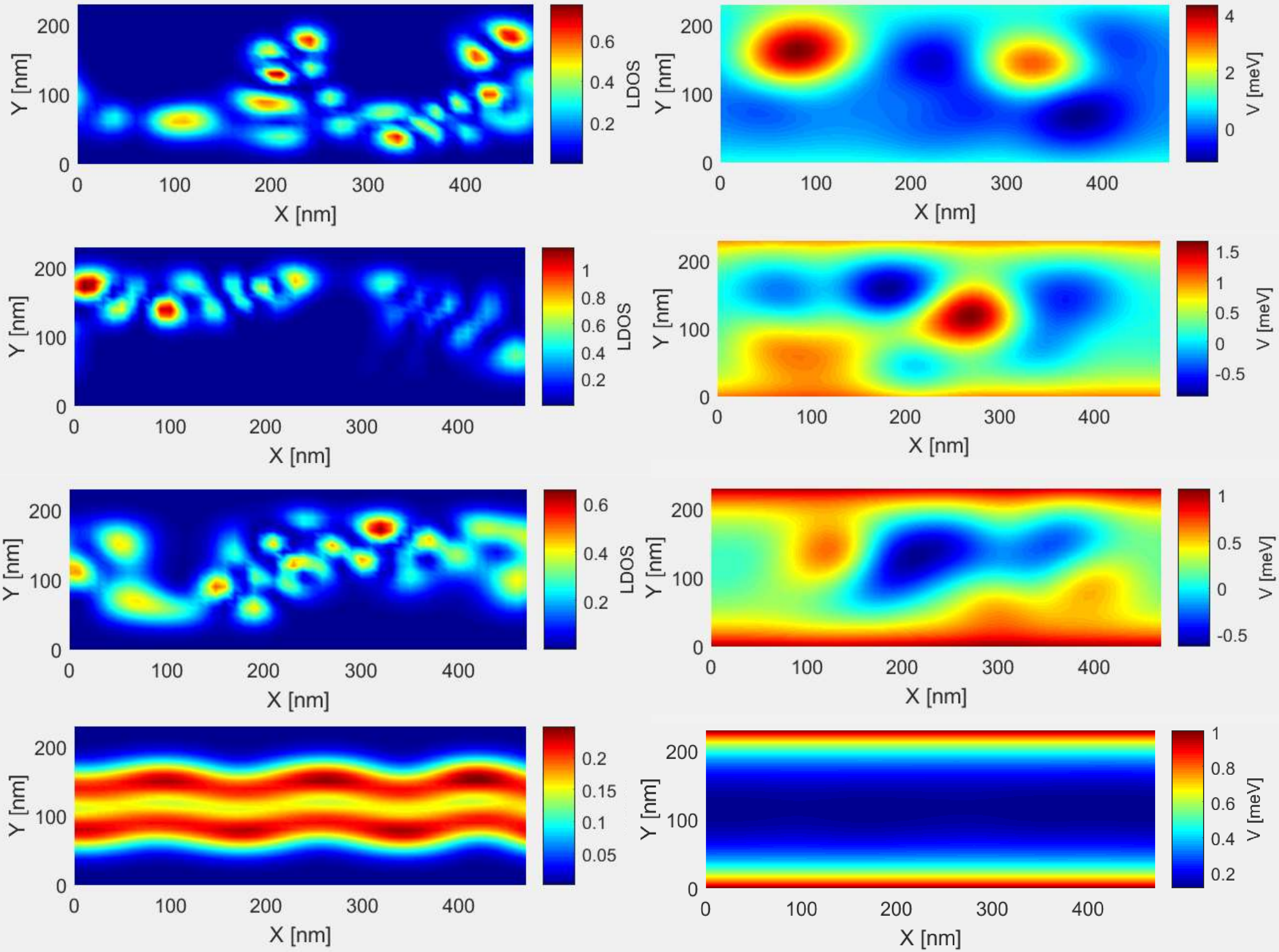
Y [nm]
200
100
0
0
100
200
300
400
X [nm]
1
0
-1
V [meV]
Easy
Hard
Y [nm]
200
100
0
0
100
200
300
400
X [nm]
0.8
0.6
0.4
0.2
LDOS

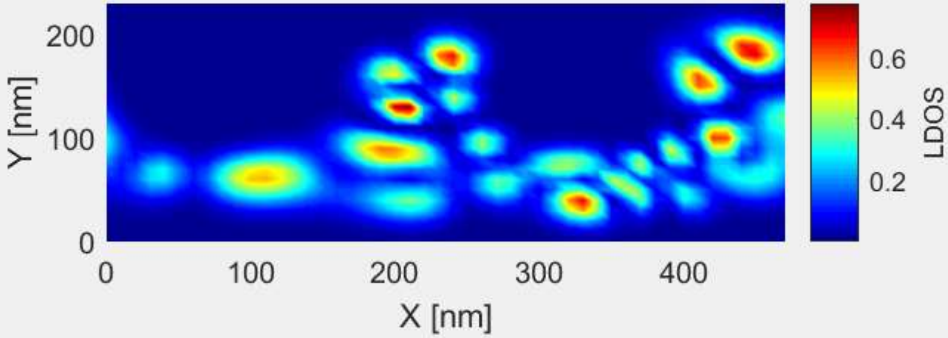


Quiz: which LDOS corresponds to the strongest disorder?

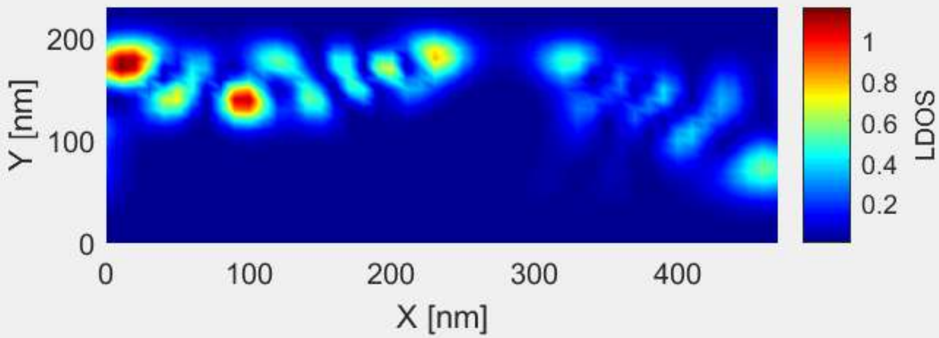


Strong disorder
Weak disorder
X [nm]
Y [nm]
LDOS
V [meV]

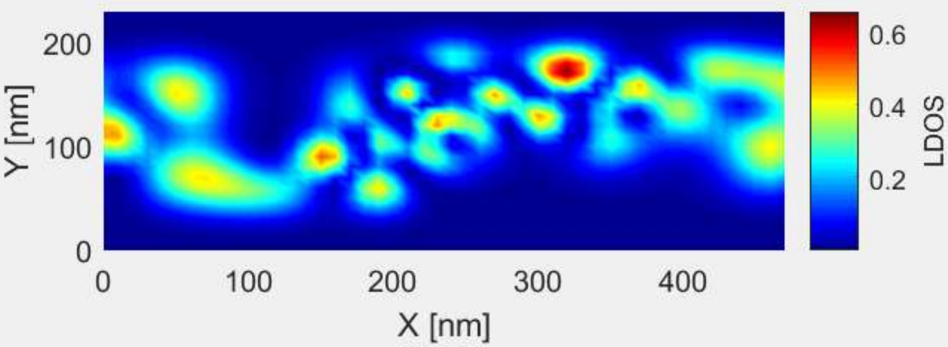

Y [nm]
X [nm]
LDOS
0.2
0.4
0.6
Y [nm]
X [nm]
V [meV]
0
2
4
Y [nm]
X [nm]
LDOS
0.2
0.4
0.6
0.8
1
Y [nm]
X [nm]
V [meV]
-0.5
0
0.5
1
1.5
Y [nm]
X [nm]
LDOS
0.2
0.4
0.6
Y [nm]
X [nm]
V [meV]
-0.5
0
0.5
1
Y [nm]
X [nm]
0.05
0.1
0.15
0.2
Y [nm]
X [nm]
V [meV]
0.2
0.4
0.6
0.8
1



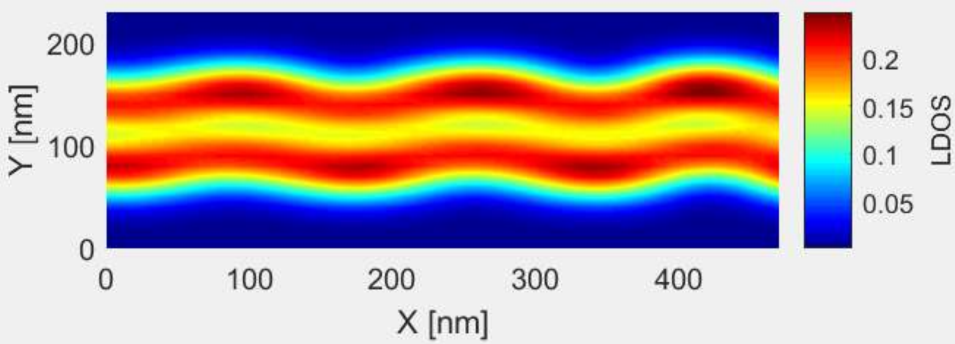
Potential 4



Potential 3

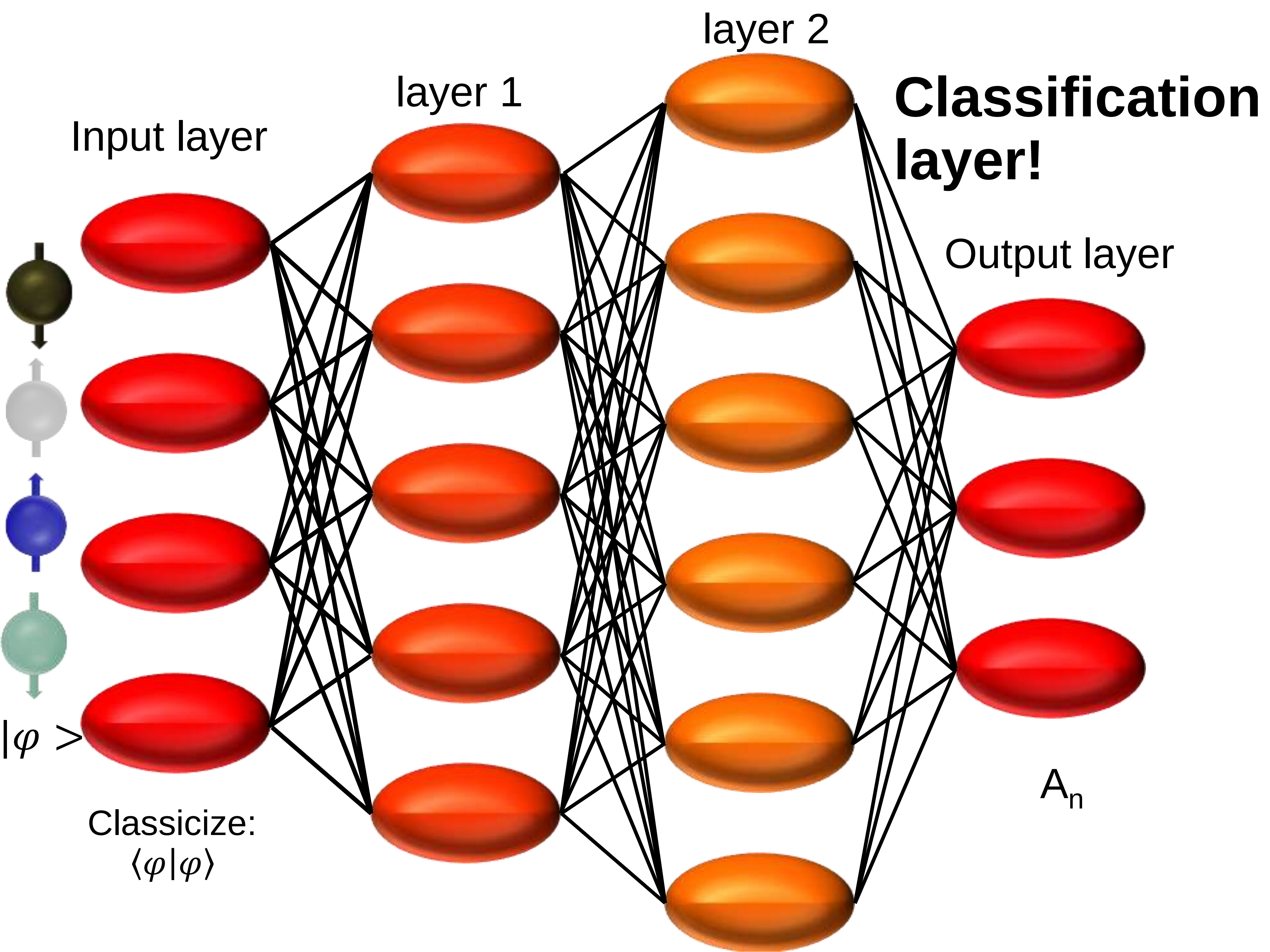


Potential 2

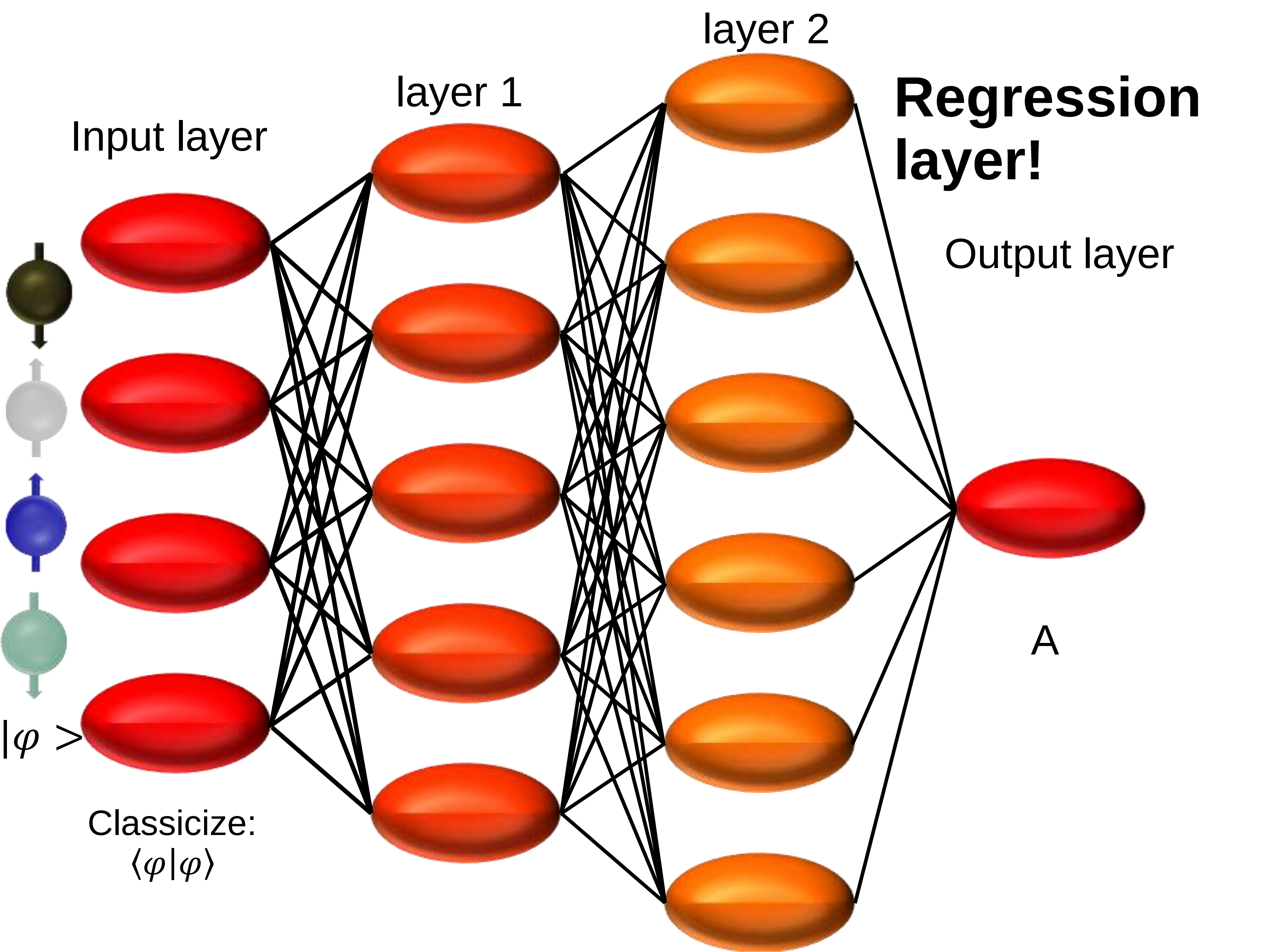


Potential 1

Matlab quantum machine learning



layer 2
layer 1
Classification layer!
Input layer
Output layer
|φ >
A_n
Classicize:
⟨φ|φ⟩

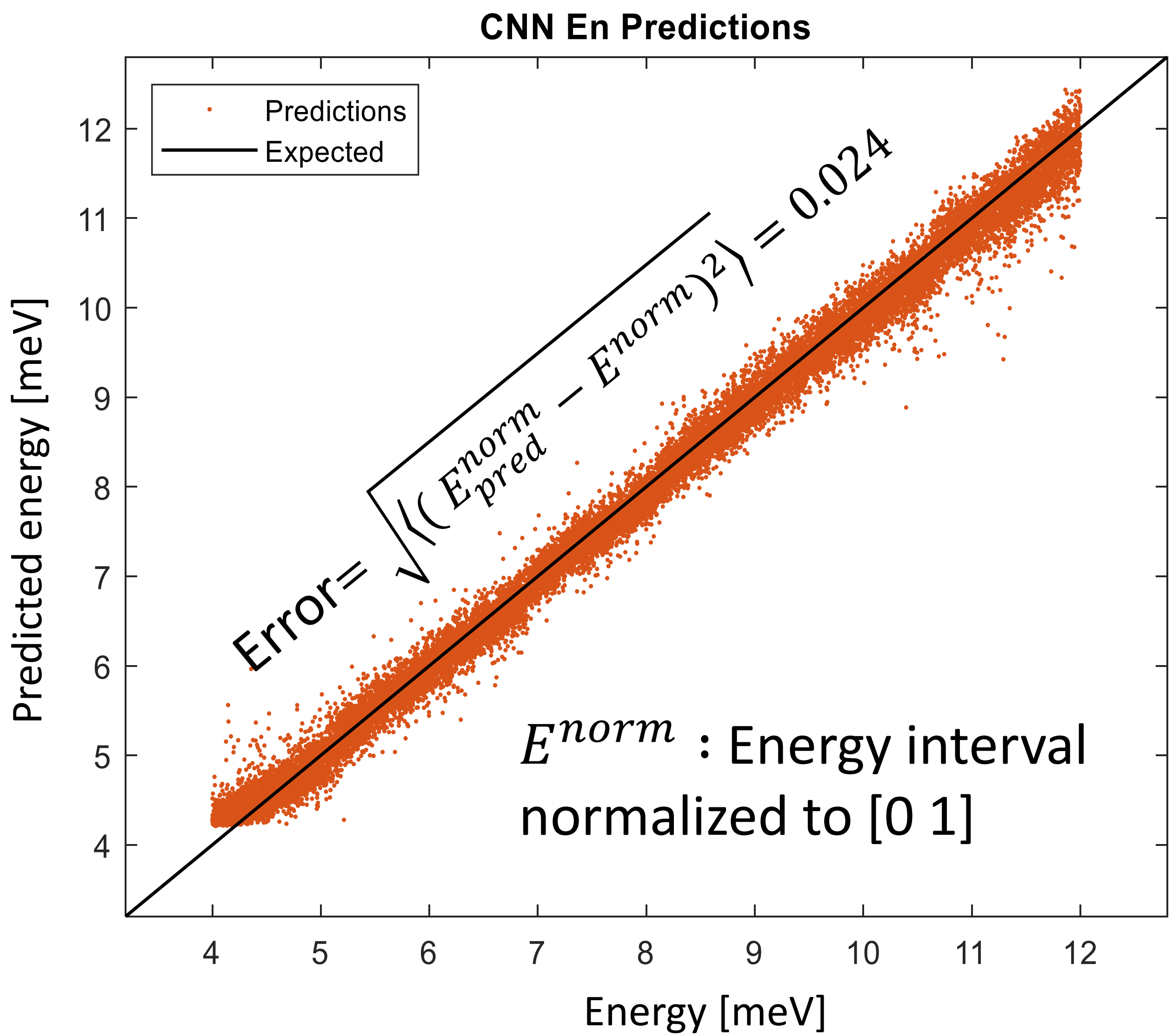

layer 2
layer 1
Regression layer!
Input layer
Output layer
A
|φ >
Classicize:
⟨φ|φ⟩

```
14x1 Layer array with layers:

   1   'imageinput'        Image Input         24x48x1 images
   2   'conv_1'            Convolution         32 5x5x1 convolutions with stride [1  1] and padding [2  2  2  2]
   3   'maxpool_1'         Max Pooling         3x3 max pooling with stride [2  2] and padding [0  0  0  0]
   4   'relu_1'            ReLU                ReLU
   5   'conv_2'            Convolution         32 5x5x32 convolutions with stride [1  1] and padding [2  2  2  2]
   6   'maxpool_2'         Max Pooling         3x3 max pooling with stride [2  2] and padding [0  0  0  0]
   7   'relu_2'            ReLU                ReLU
   8   'conv_3'            Convolution         64 5x5x32 convolutions with stride [1  1] and padding [2  2  2  2]
   9   'maxpool_3'         Max Pooling         3x3 max pooling with stride [2  2] and padding [0  0  0  0]
  10   'relu_3'            ReLU                ReLU
  11   'fc_1'              Fully Connected     100 fully connected layer
  12   'relu_4'            ReLU                ReLU
  13   'fc_2'              Fully Connected     1 fully connected layer
  14   'regressionoutput'  Regression Output   mean-squared-error with response 'Response'
```

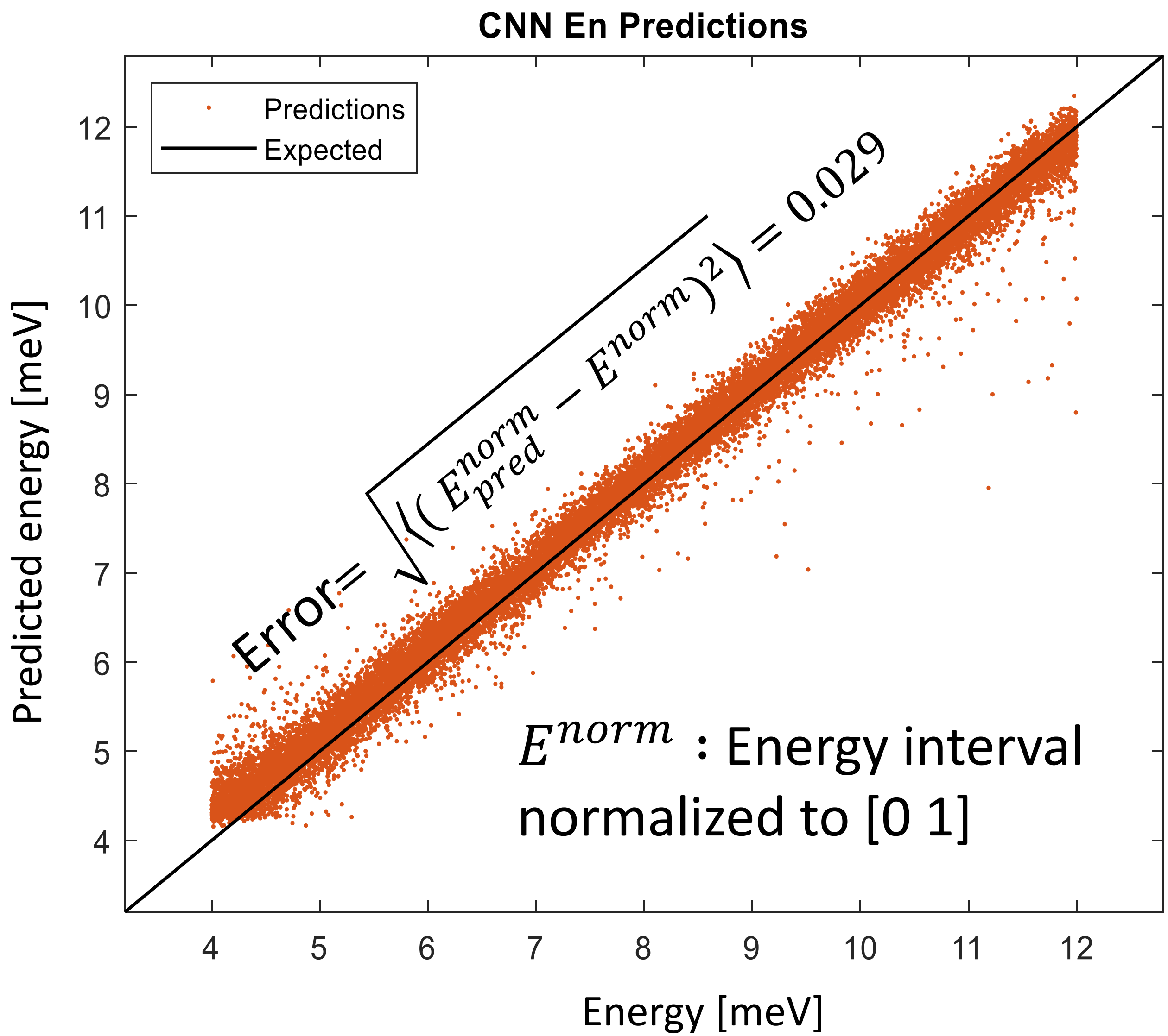
Regression result: B=0

(100k images; 20k predictions)



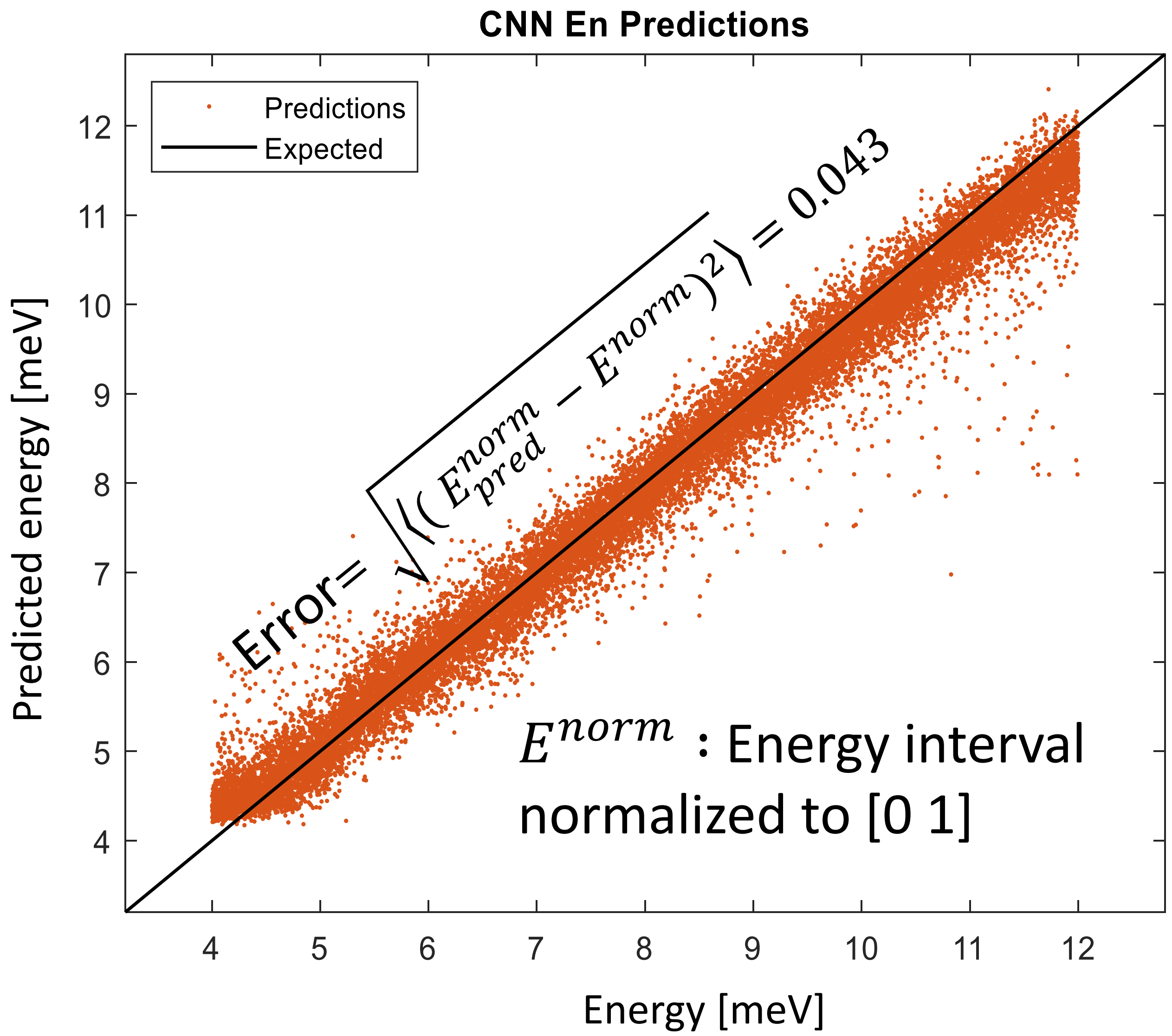
Regression result: B=1T

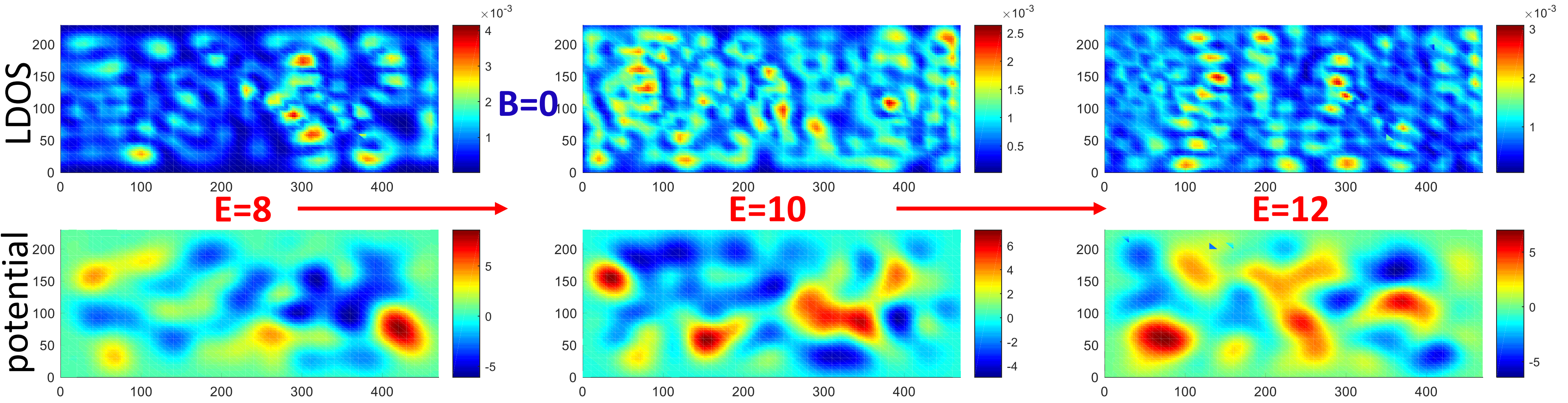
(100k images; 20k predictions)



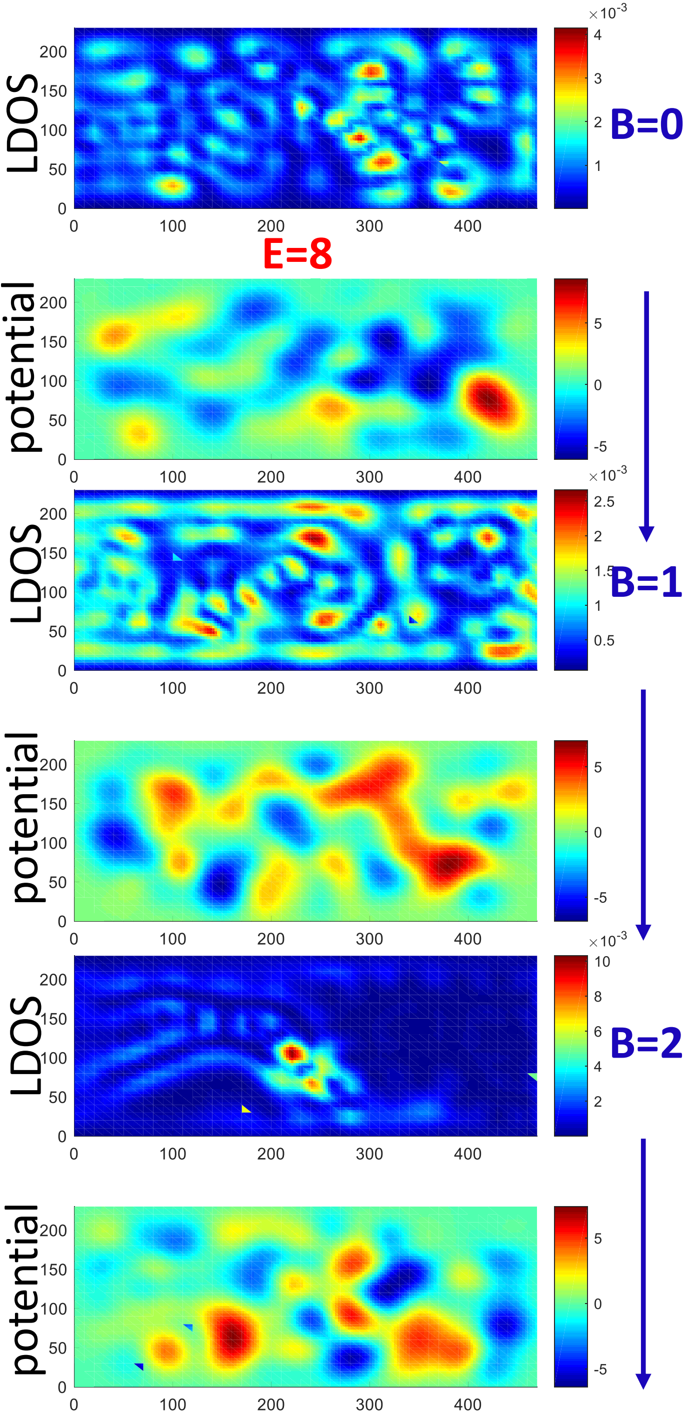
Regression result: B=2T

(100k images; 20k predictions)

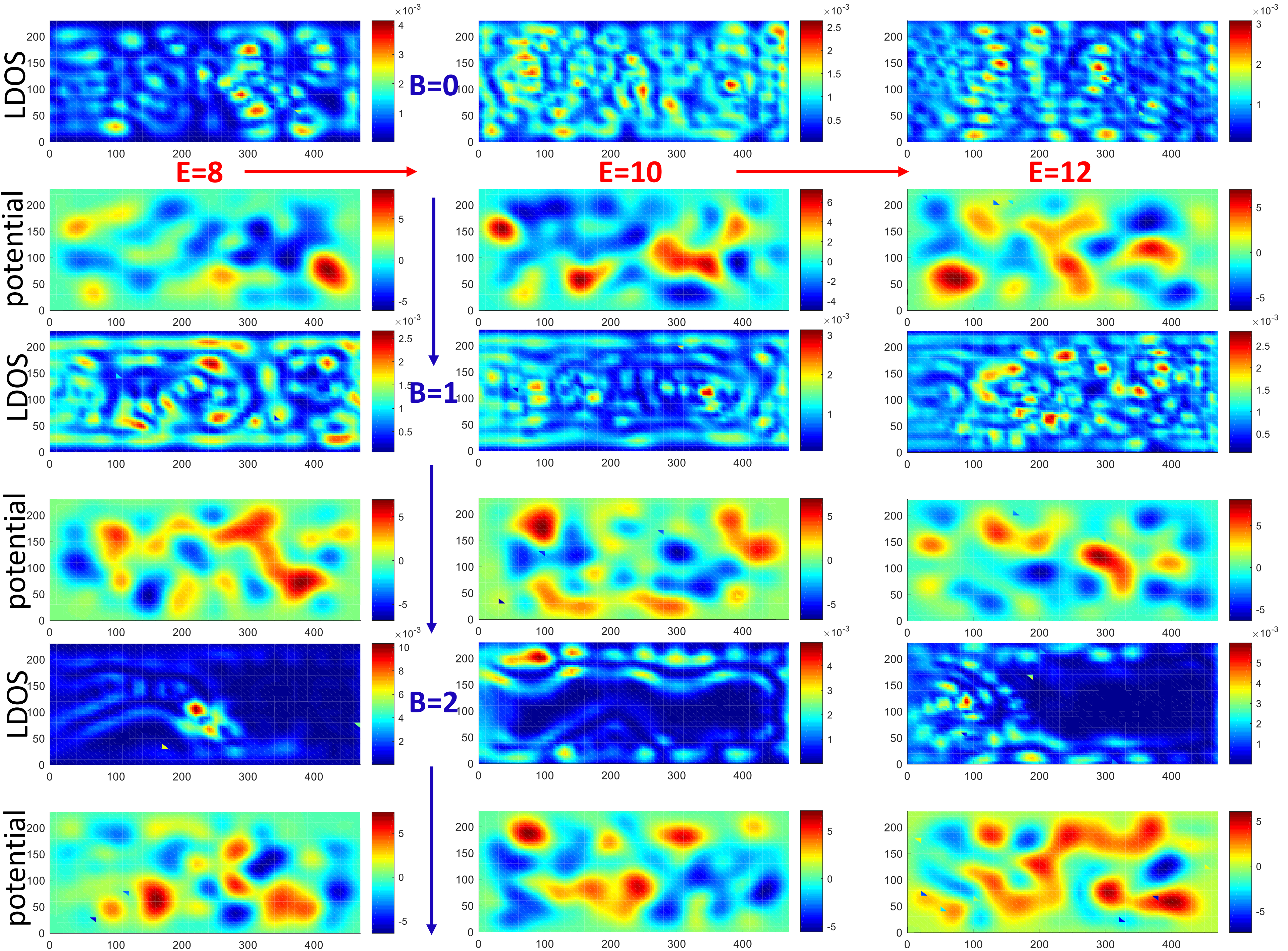




LDOS
potential
B=0
E=8
E=10
E=12



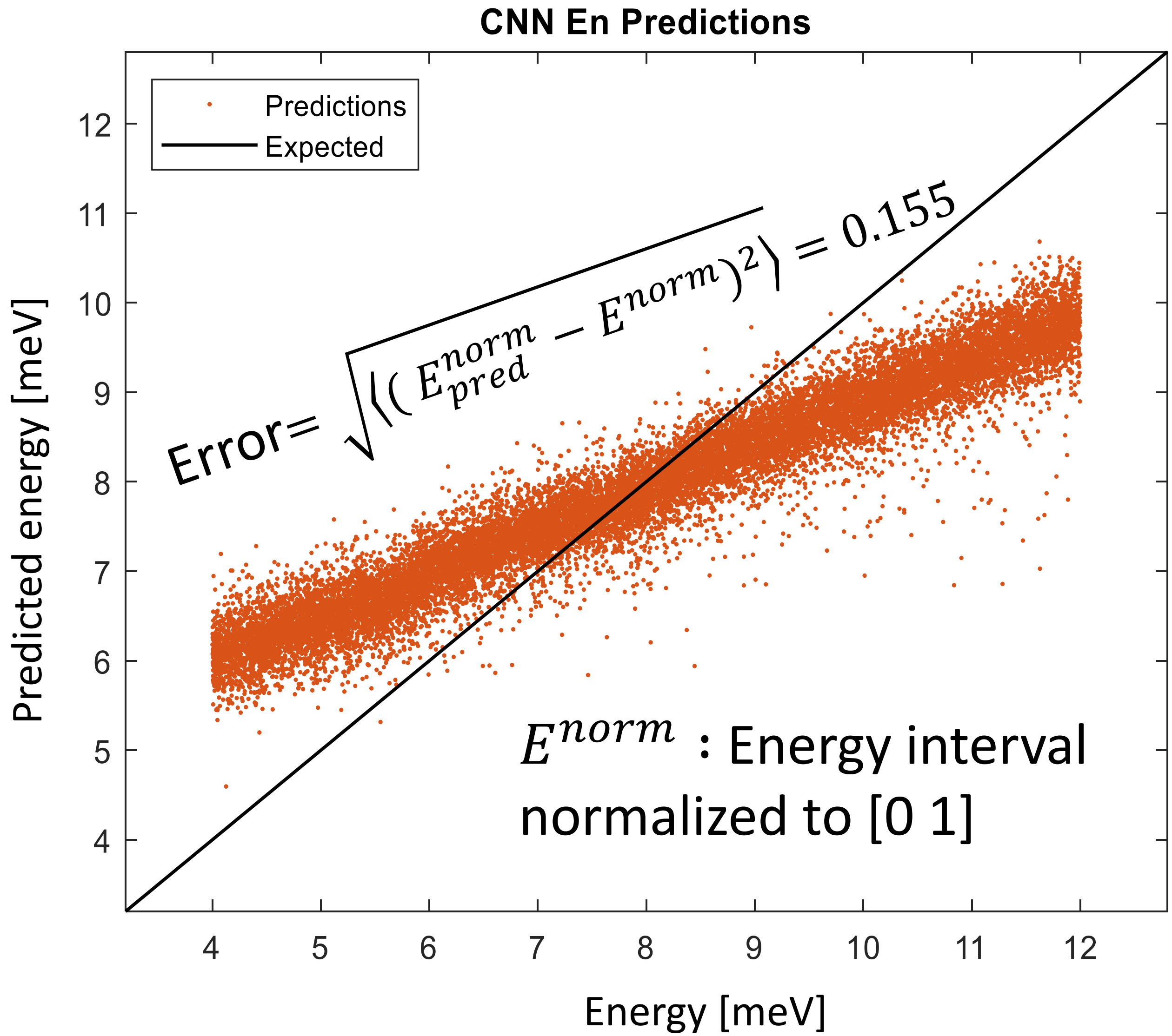
LDOS
B=0
E=8
potential
LDOS
B=1
potential
LDOS
B=2
potential



LDOS
B=0
E=8
E=10
E=12
potential
LDOS
B=1
potential
LDOS
B=2
potential

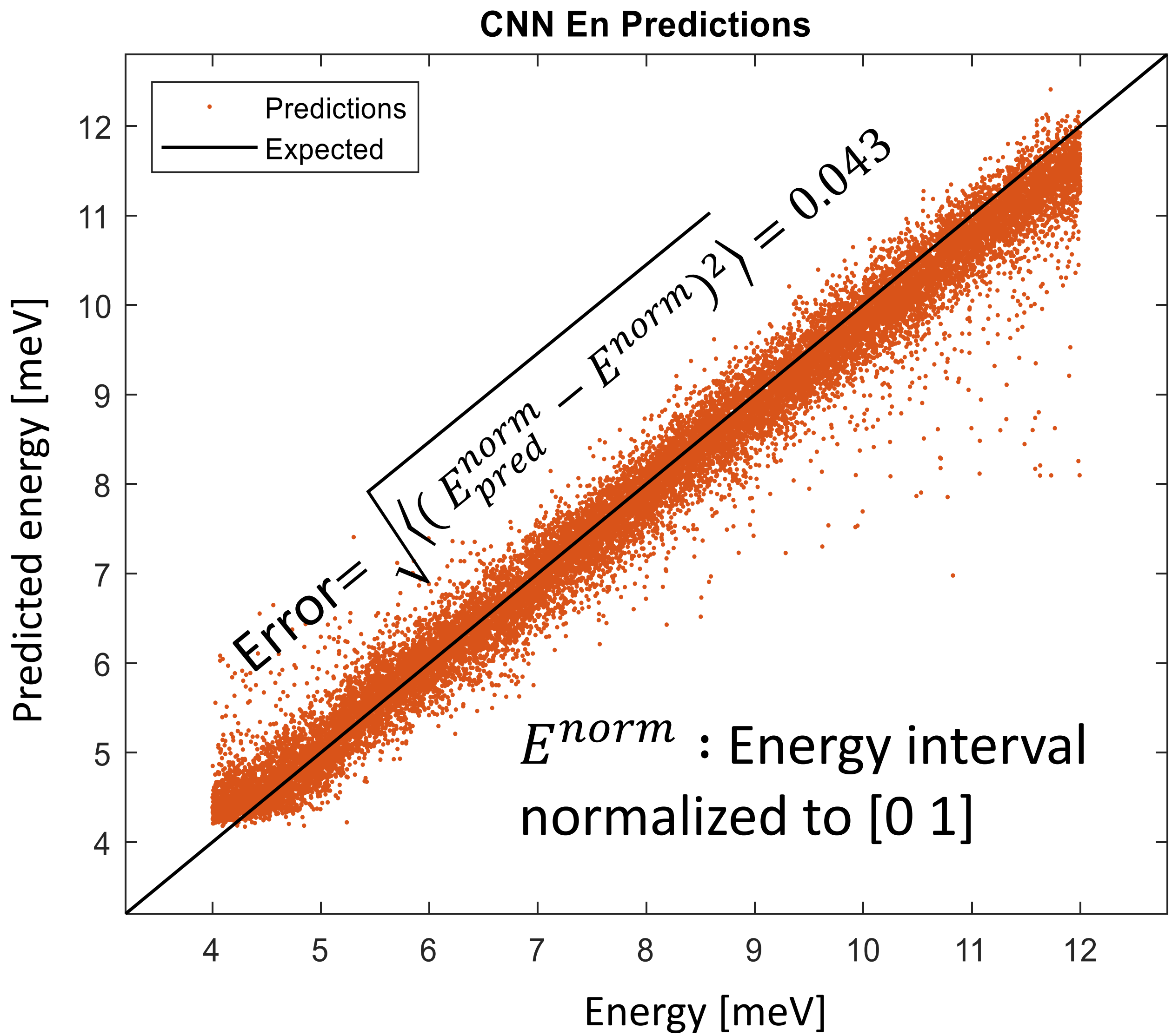
Regression result: trained at B=2T -> prediction with B=1T

(100k images; 20k predictions)



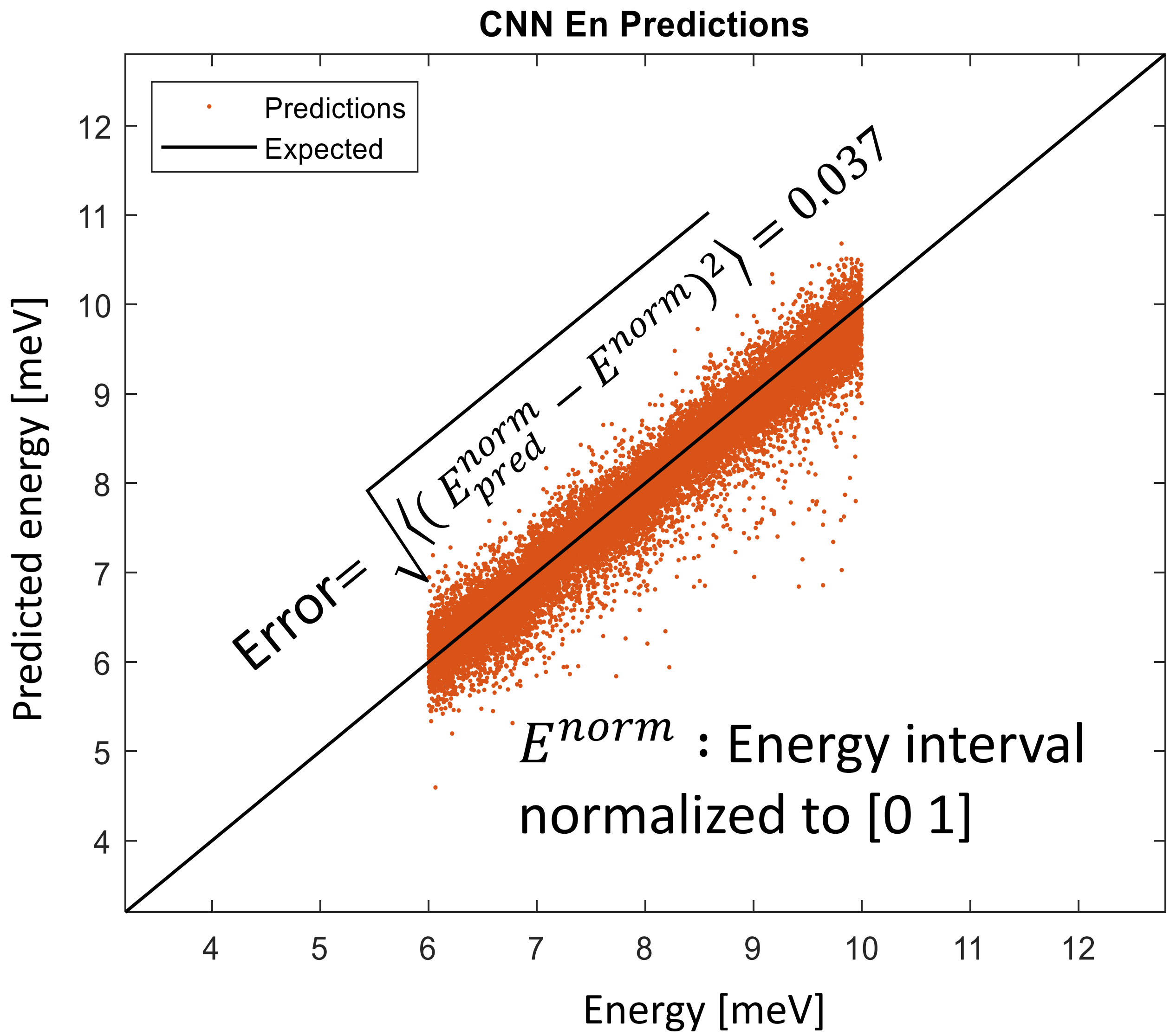
Regression result: B=2T

(100k images; 20k predictions)



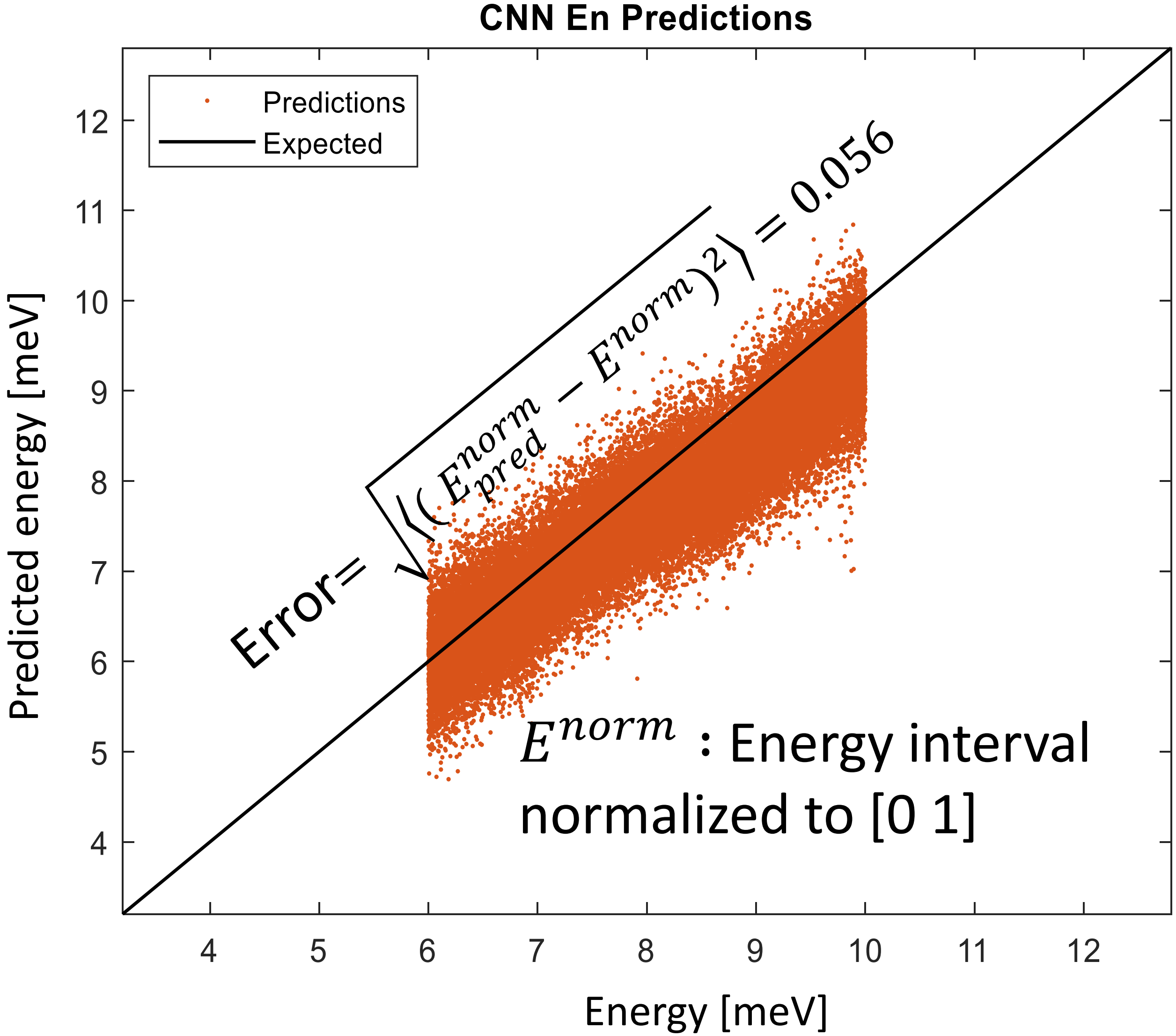
Regression result: B=2T (tested on smaller range)

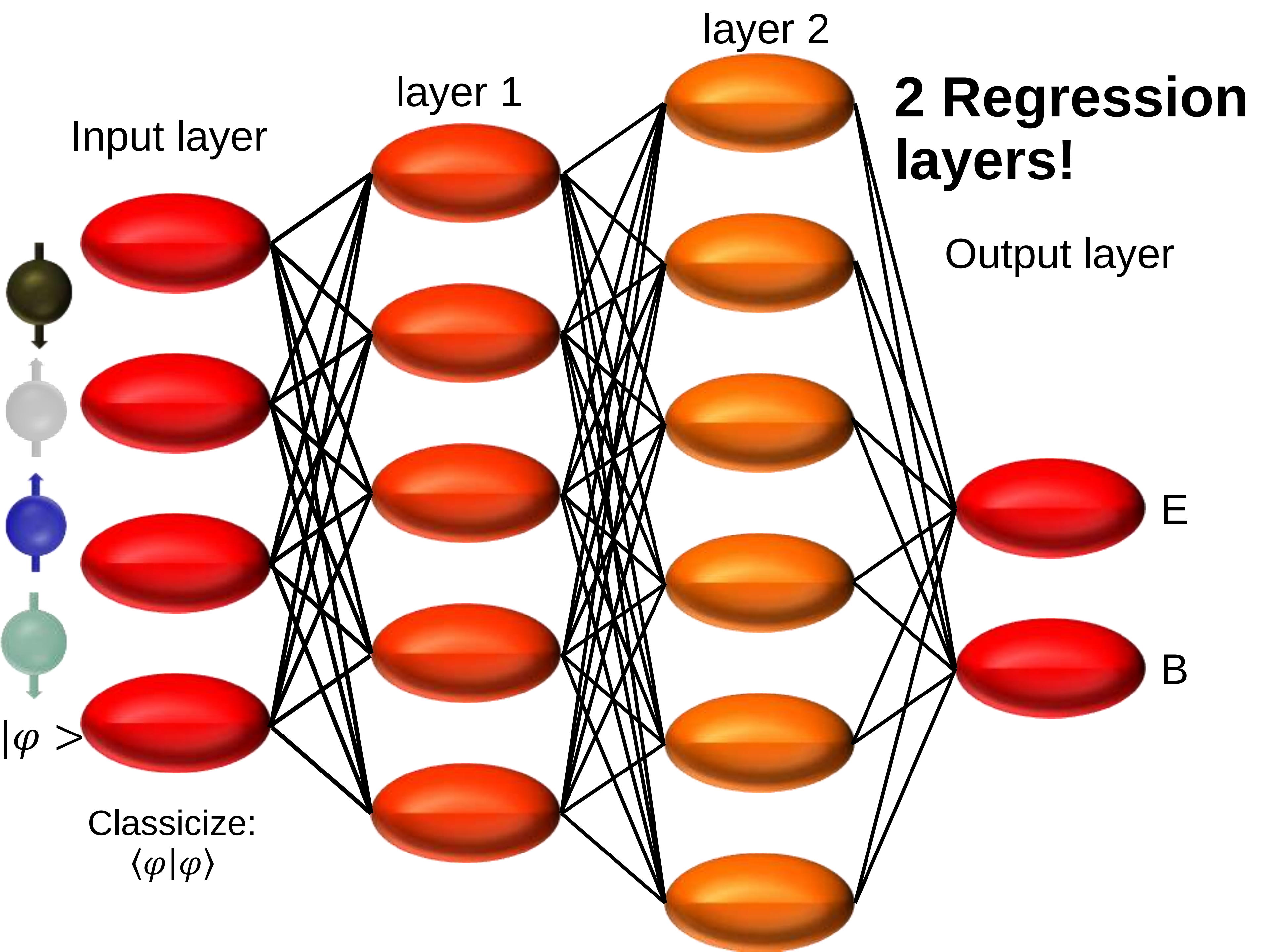
(100k images; 20k predictions)



Regression result: B=2T (trained on smaller range)

(100k images; 20k predictions)



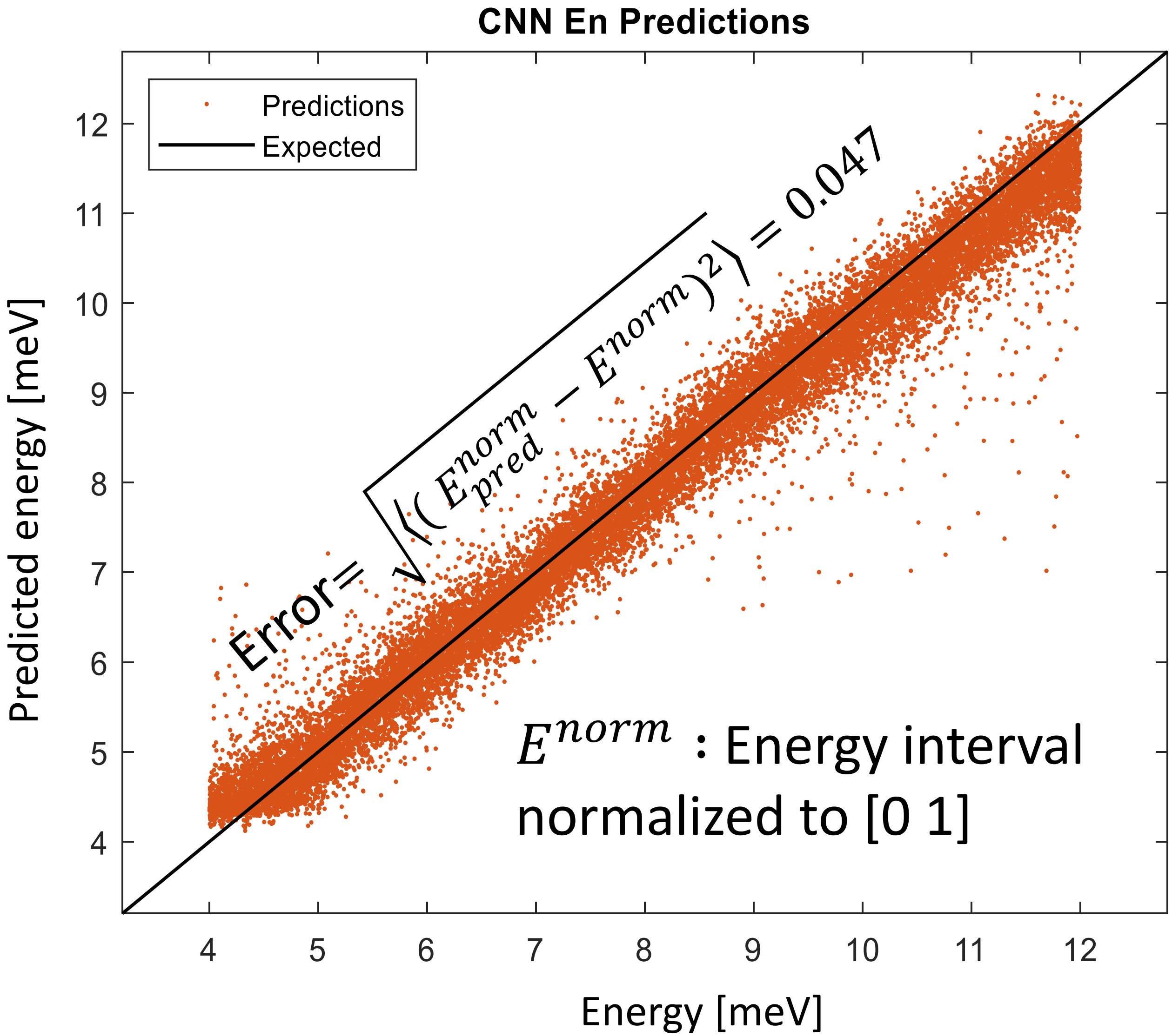


layer 2
layer 1
2 Regression layers!
Input layer
Output layer
E
B
$|\varphi >$
Classicize:
$\langle\varphi|\varphi\rangle$

Regression result: B=[1-3]T (Training B and E simultaneously)

2 regressions

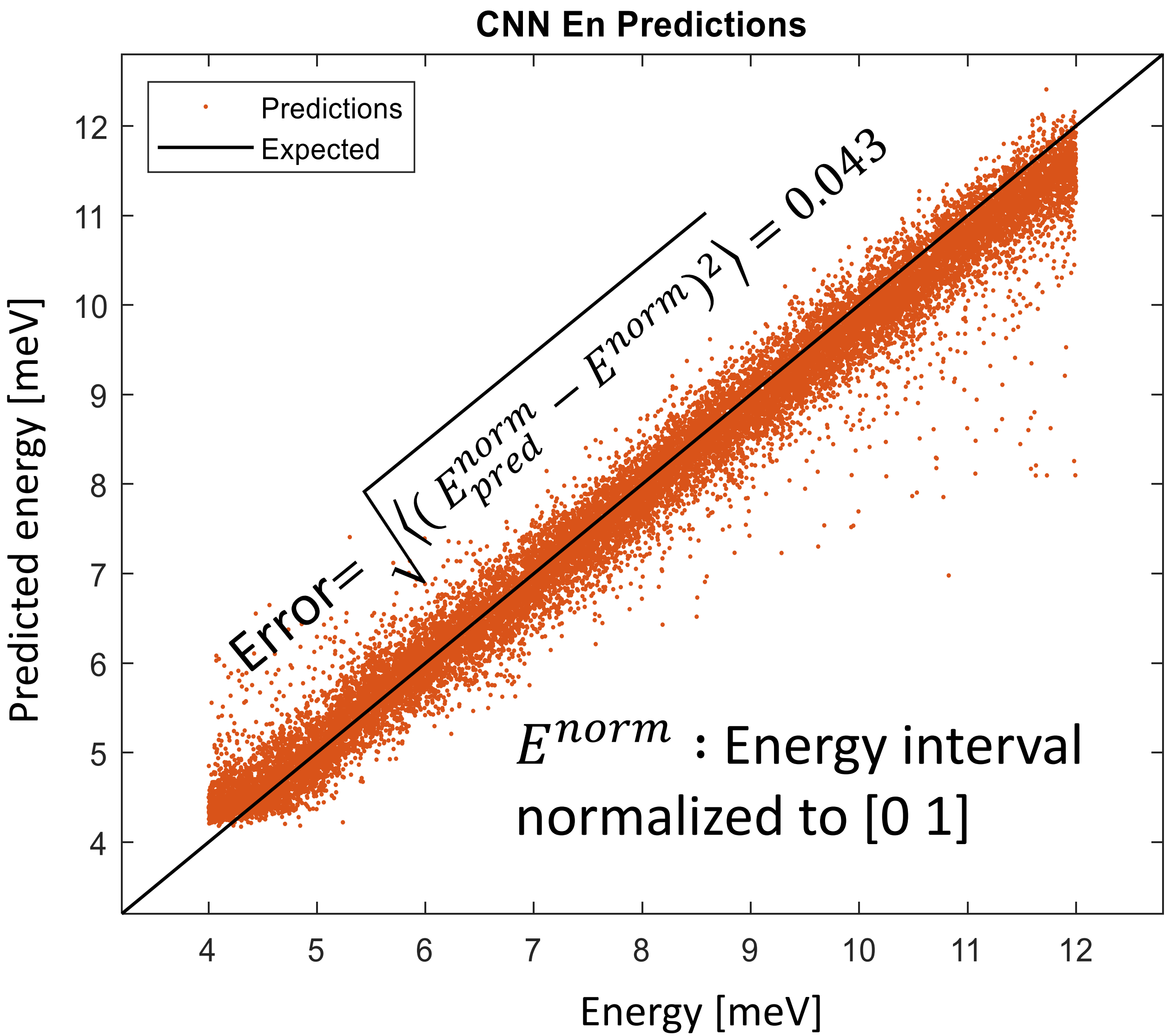
(100k images; 20k predictions)



Regression result: B=2T (Training only E)

(100k images; 20k predictions)

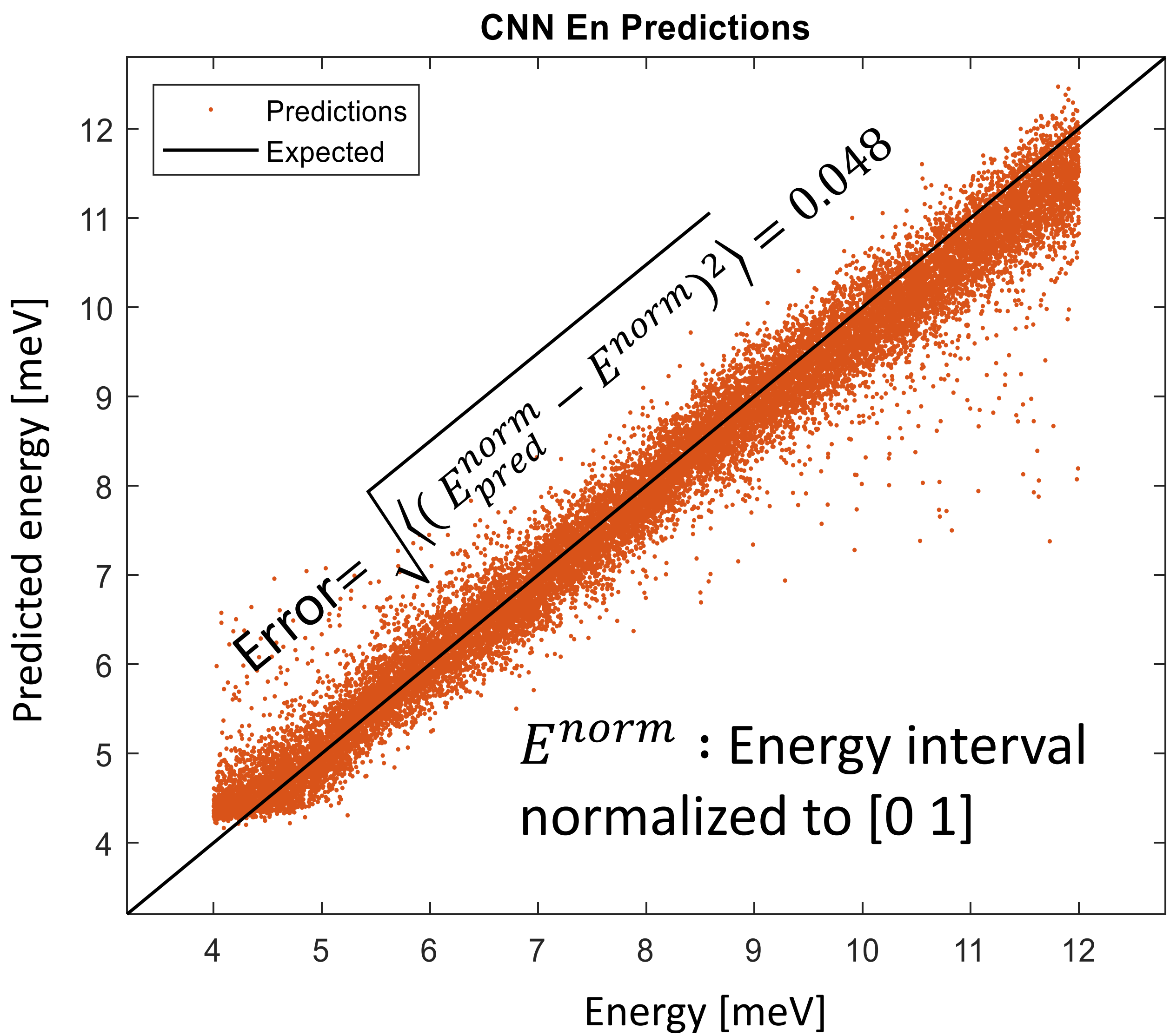
1 regression

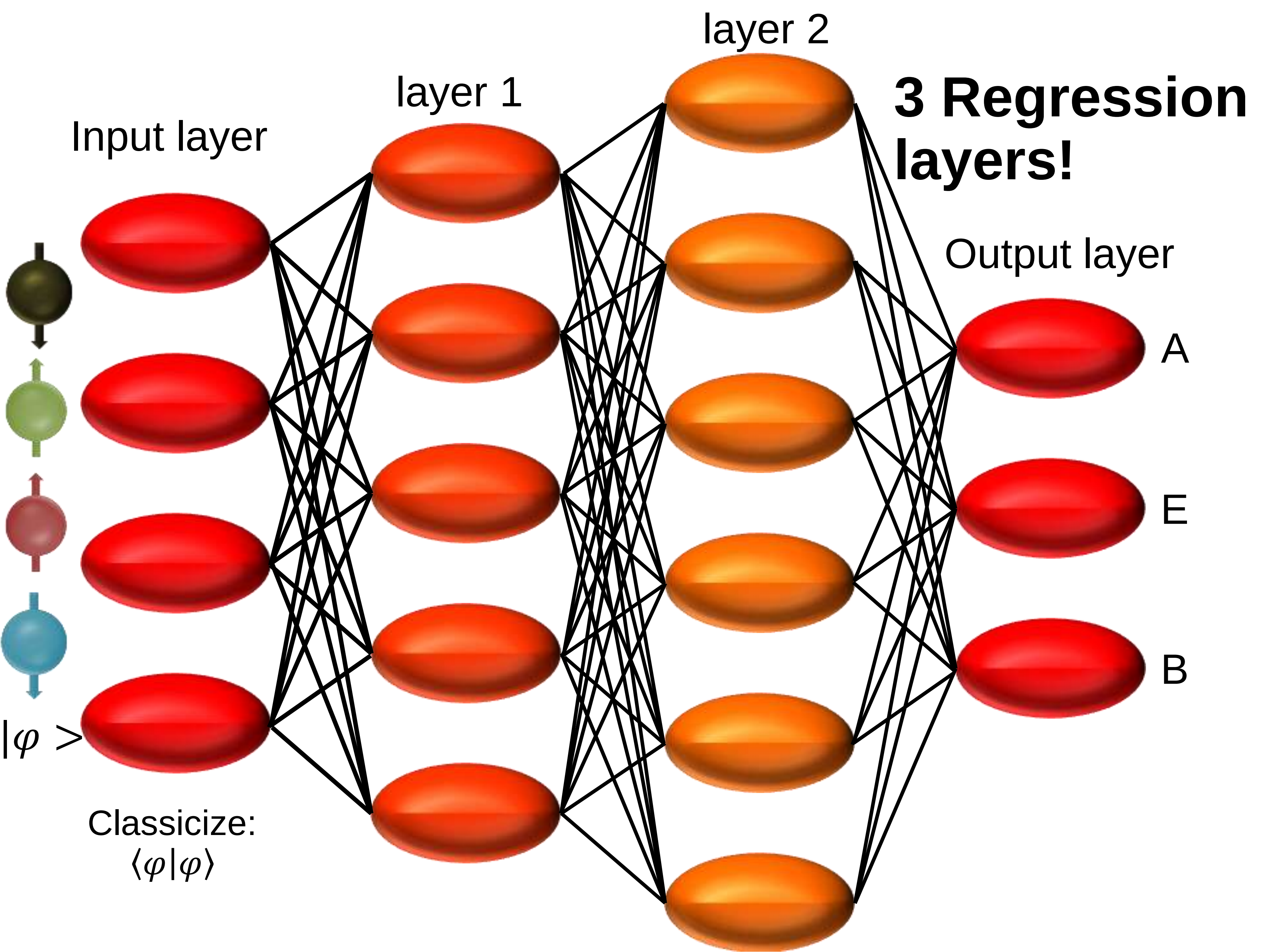


Regression result: Prediction for B=2T (trained for B=[1-3]T)

2 regressions

(100k images; 20k predictions)



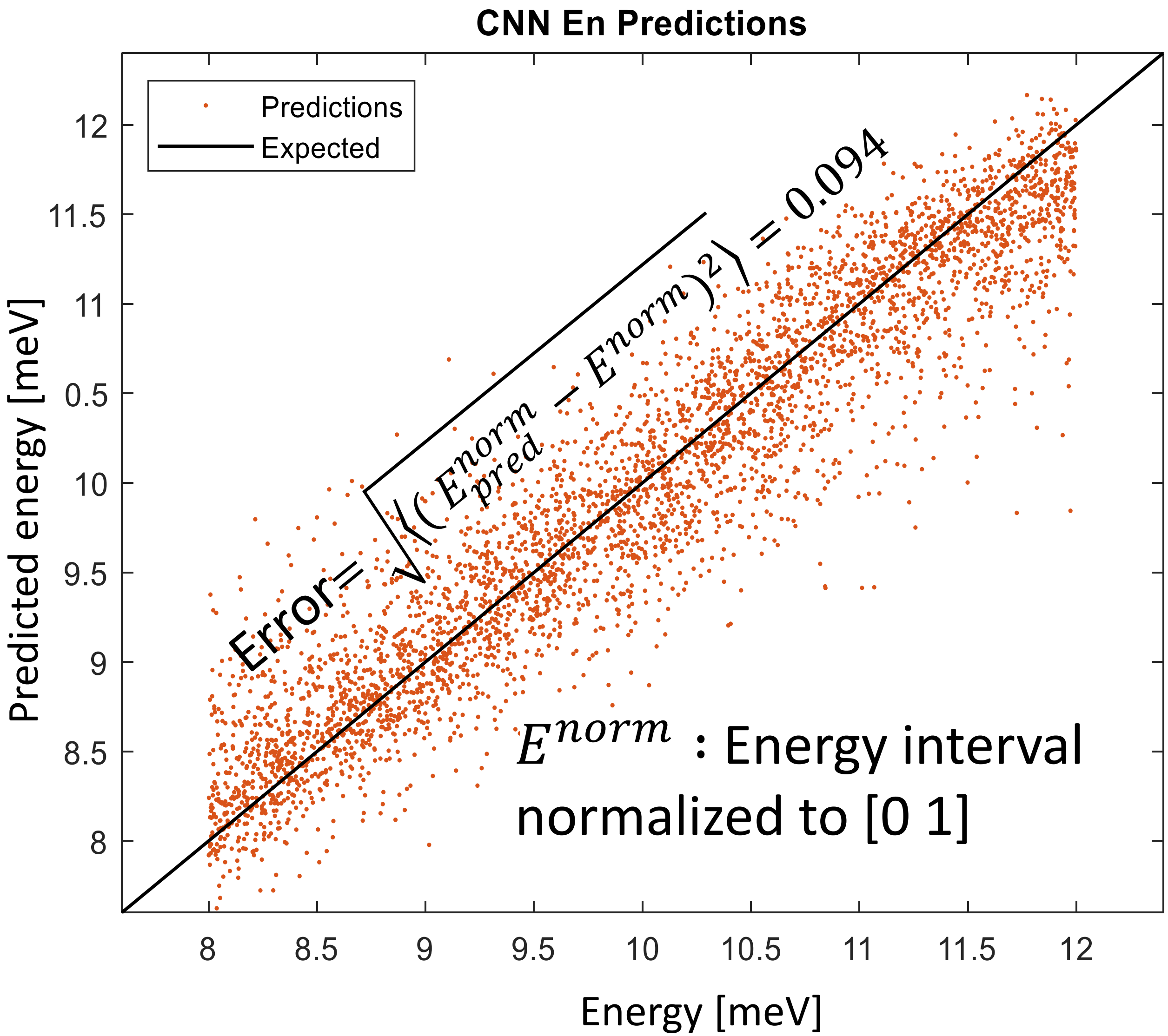


layer 2
layer 1
3 Regression layers!
Input layer
Output layer
A
E
B
|φ >
Classicize:
⟨φ|φ⟩

Regression result: B=[1.25-2]T; A=[0-5]; E=[8-12] (training and prediction)

3 regressions

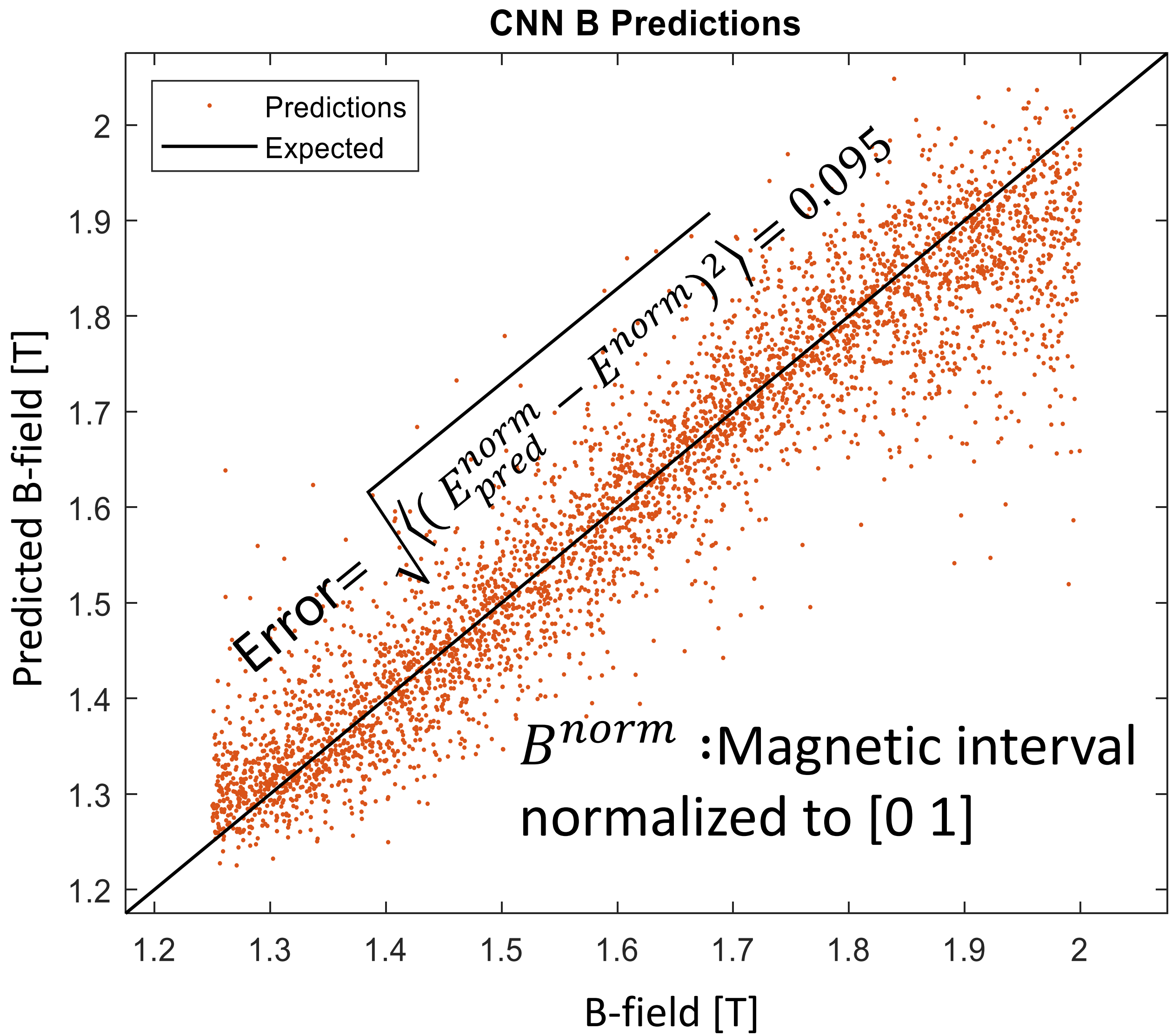
(20k images; 4k predictions)



Regression result: B=[1.25-2]T; A=[0-5]; E=[8-12] (training and prediction)

3 regressions

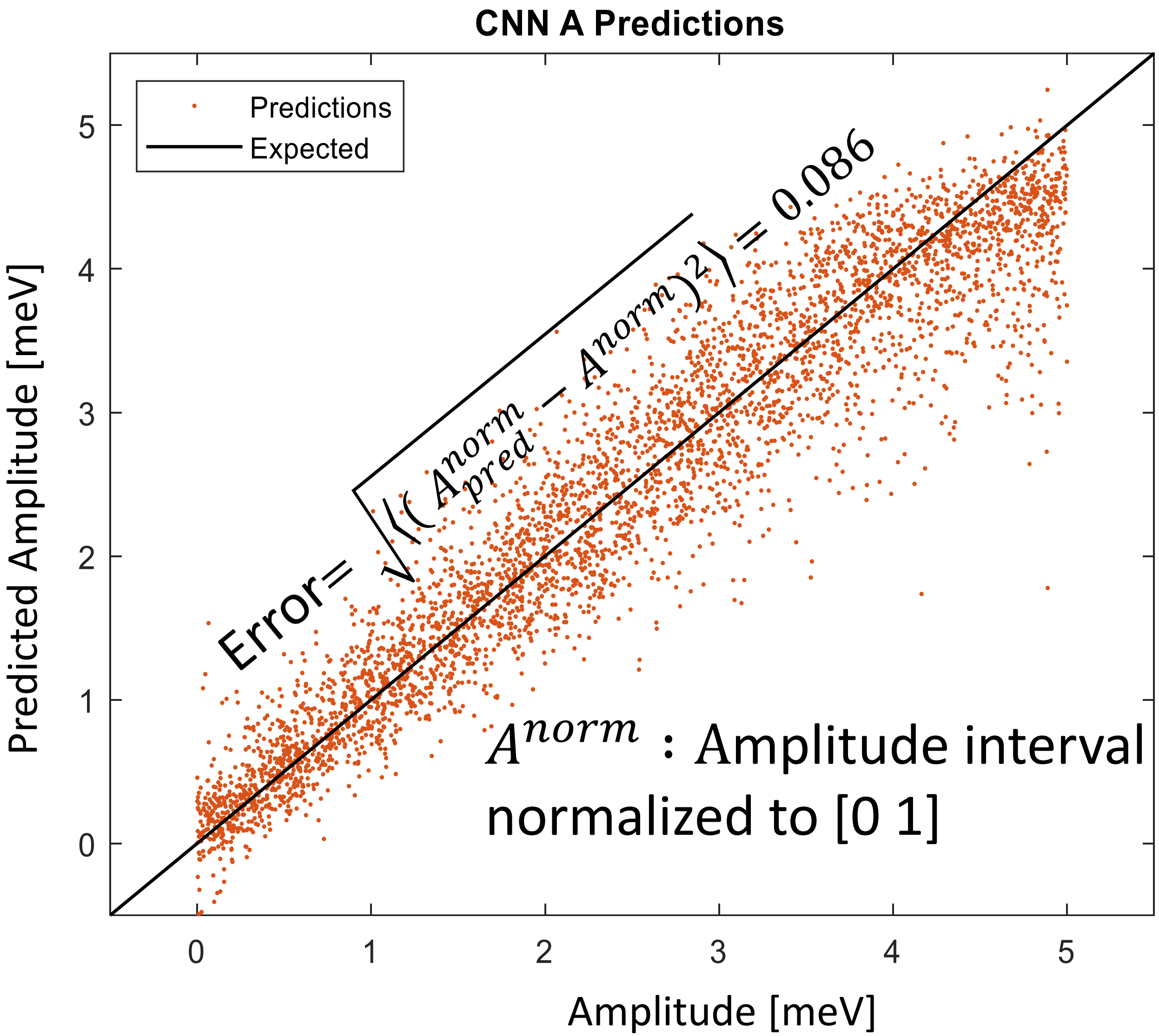
(20k images; 4k predictions)



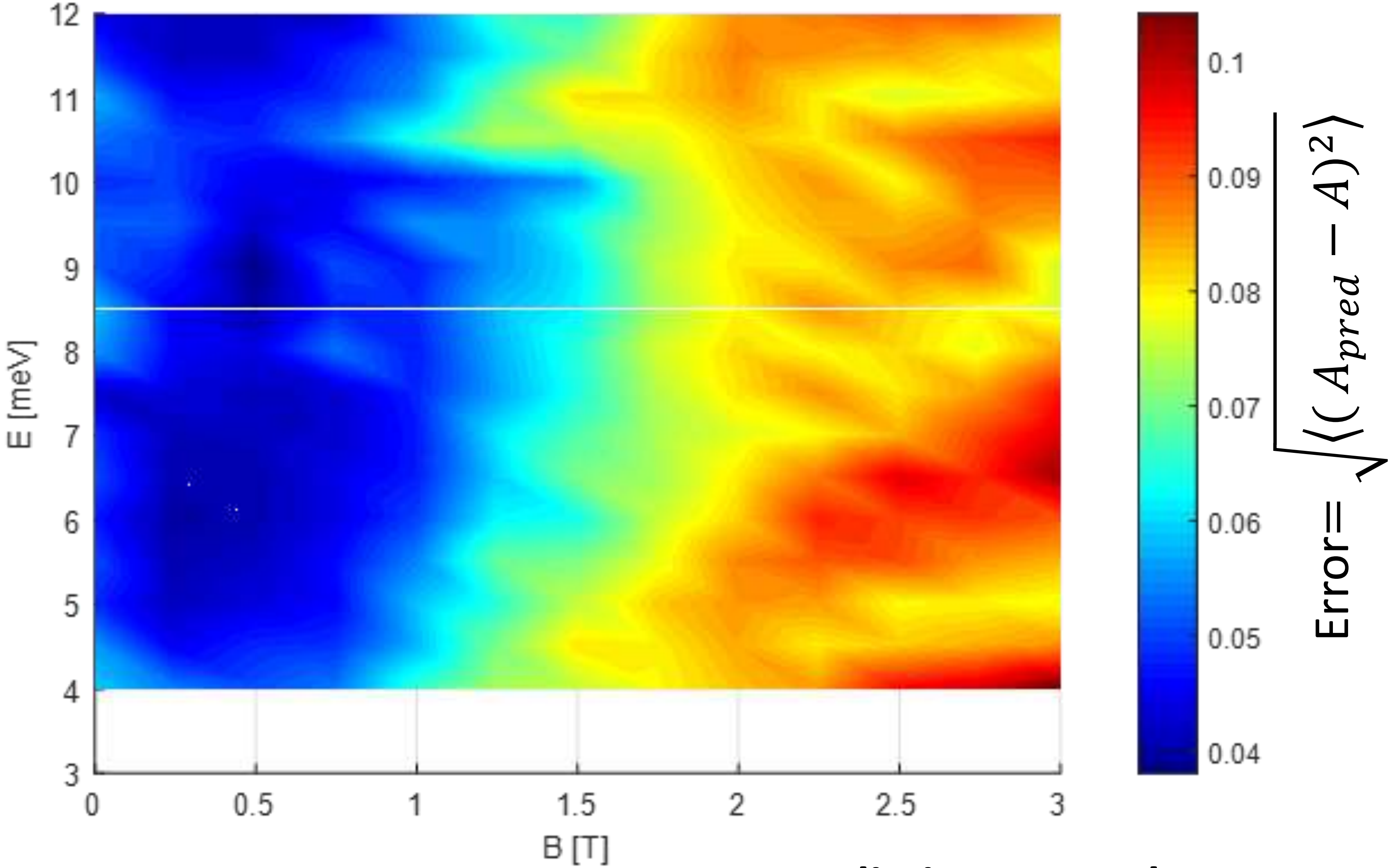
Regression result: B=[1.25-2]T; A=[0-5]; E=[8-12] (training and prediction)

3 regressions

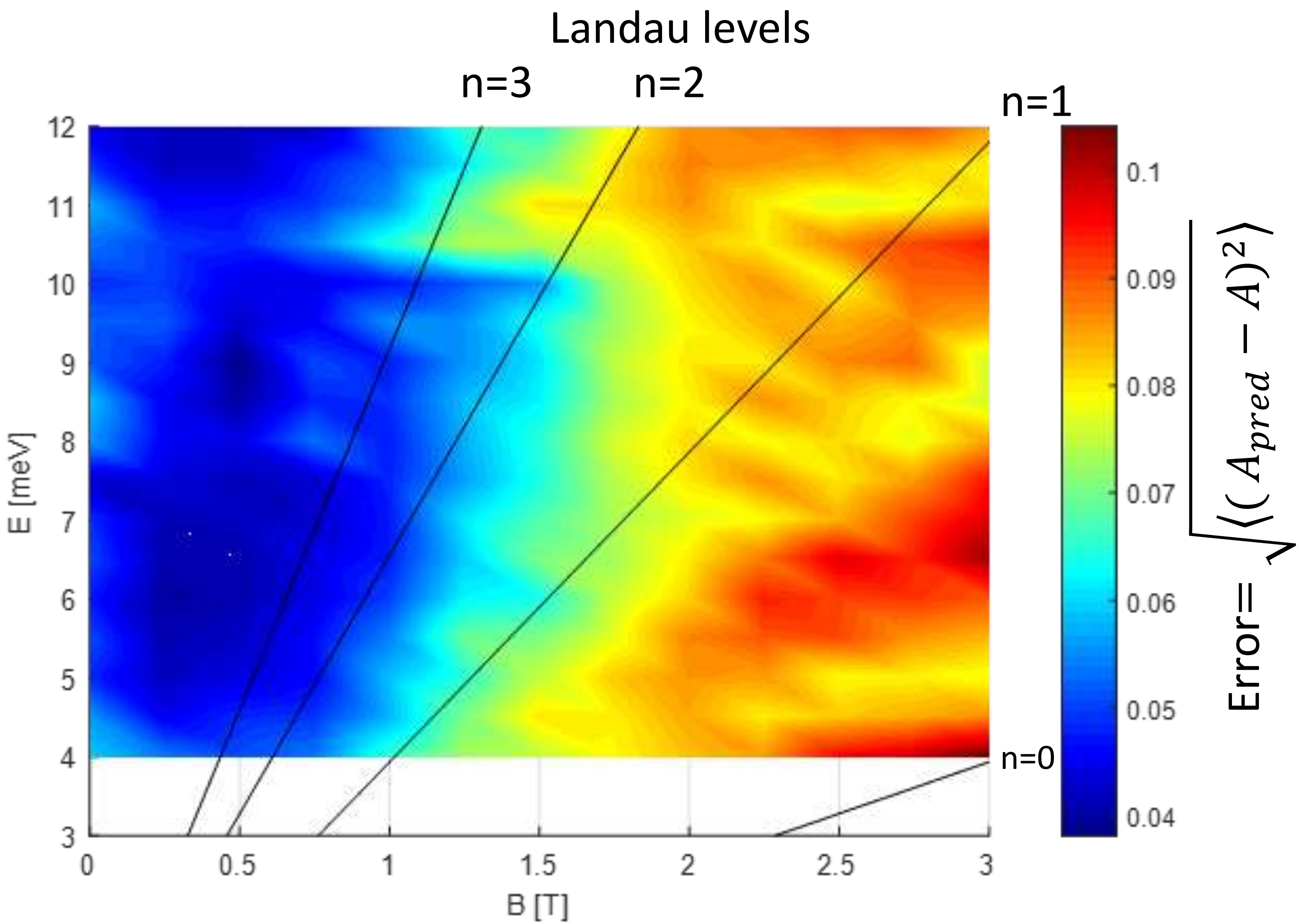
(20k images; 4k predictions)



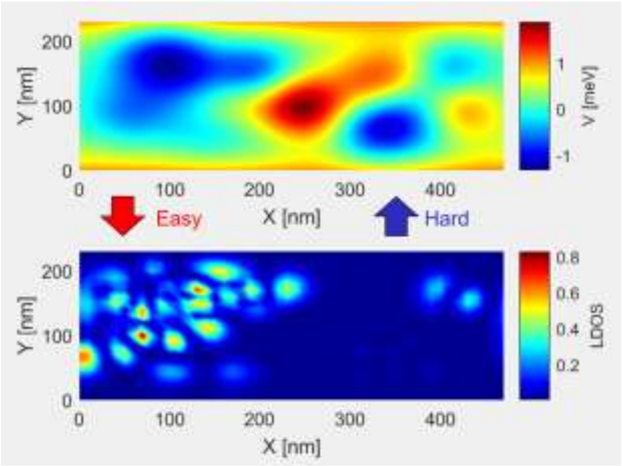
Error of A (amplitude) prediction as a function of B (magnetic field) and E (energy)



Prediction error phase space



Landau levels
n=3
n=2
n=1
n=0
12
11
10
9
8
7
6
5
4
3
E [meV]
0
0.5
1
1.5
2
2.5
3
B [T]
0.1
0.09
0.08
0.07
0.06
0.05
0.04
Error= $\sqrt{\langle (A_{pred} - A)^2 \rangle}$



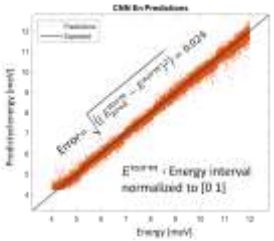
Potential

LDOS

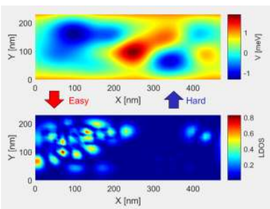
The network can learn B (magnetic field), A (amplitude) and E (energy) simultaneously.

We pushed it to 5 additional parameters: depletion width, correlation length, impurity shape (Gaussian vs. Lorentzian), impurity sharpness, and impurity density and the NN can learn all 8 (not all equally well).

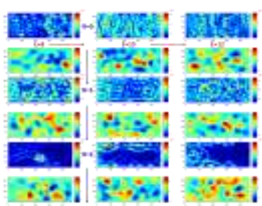
(Quantum) machine learning conclusions:



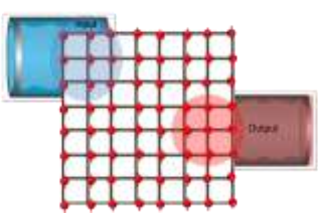
- Regression machine learning algorithms are much more effective than classification ones. Can be extended to learn many variables.



- Quantum states are an ideal playground to apply classical machine learning. Can be applied to many systems, but disordered systems are particularly attractive due to disorder averaging which gives large training data. Can solve some new and old problems much more efficiently.



- Quantum states are very effective for optimizing classical machine learning networks because of the ability to generate large learning data.



- Next frontier in quantum states –quantum machine learning coming…

Thanks!