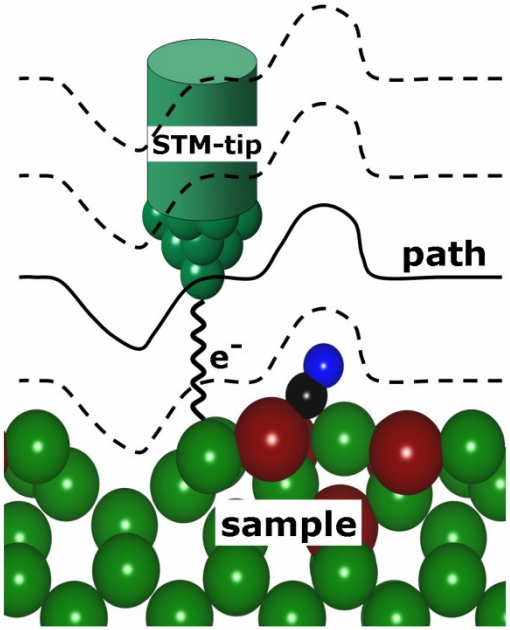
university of groningen
faculty of philosophy

March 2011, All models are wrong

Models in Material Physics

Two cases without error bars



Sylvia Wenmackers, Danny E.P. Vanpoucke
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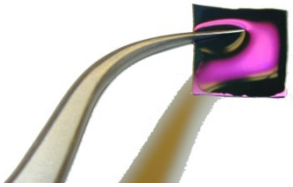
I.
A.
B.
II.
A.
B

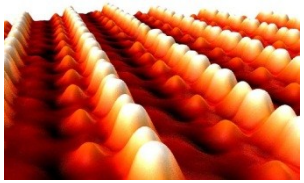
Structure of talk

Scientific models

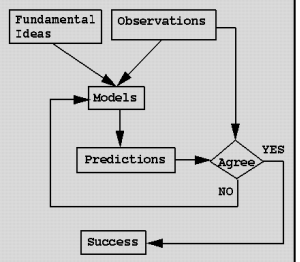
Concepts from philosophy of science

Case 1 

Ellipsometry of DNA on diamond

Case 2 

STM of nanowires on Ge(001)



Philosophy of scientific models

Semantics of models

What do models represent?

Epistemology of models

How can we learn from models?

Ontology of models

What are models?

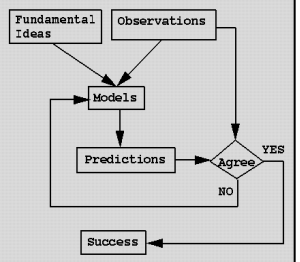
Statistics

- Mathematical models
- Models of data

Material physics

- Material sample

Frigg&Hartmann in: Sarkar&Pfeifer *Phil of Sci: Encycl.* (2005)



Philosophy of scientific models

What do models represent?

World

Target system

- phenomena
- data

Not exclusive

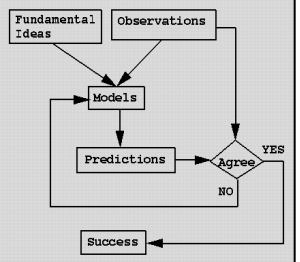
Theory

Model

- Model of phenomena
- Model of data

& curve-fitting problem

Frigg&Hartmann in: Sarkar&Pfeifer *Phil of Sci: Encycl.* (2005)



Philosophy of scientific models

How can we learn from models?

1) Denotation

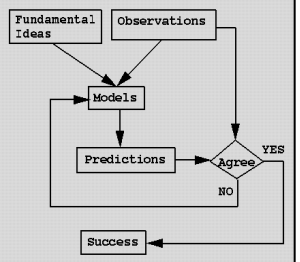
World ⇄ Model

2) Demonstration: learn, predict,…

3) Interpretation

Learning via model happens in 3 steps

R.I.G. Hughes *Philosophy of Science* **64** (1997) S325-336



Philosophy of scientific models

What are models?

1) Denotation

World ⇄ **Model**

2) Demonstration: learn, predict,…

3) Interpretation

Not exclusive

Material (Iconic)

- Scaled-up or scaled-down
- Sample

Ideal

- Thought experiments
- Descriptions
- Mathematical models

Frigg&Hartmann in: Sarkar&Pfeifer *Phil of Sci: Encycl.* (2005)

Ellipsometry of DNA on diamond

Introduction of case

research question, method, and result

How reliable is the result?

Analyze experiment & calculation

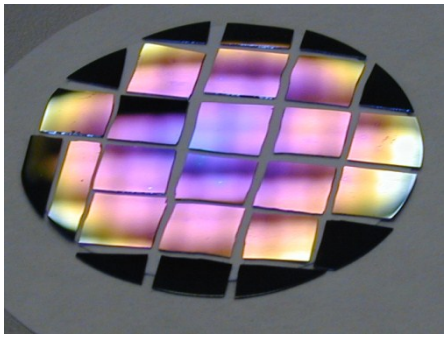
-Complex process

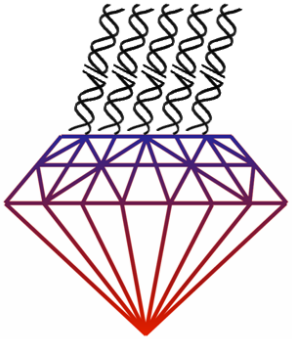
-Different types of theories & models

-Possibility of errors at each stage

Conclusion

Ellipsometry of DNA on diamond





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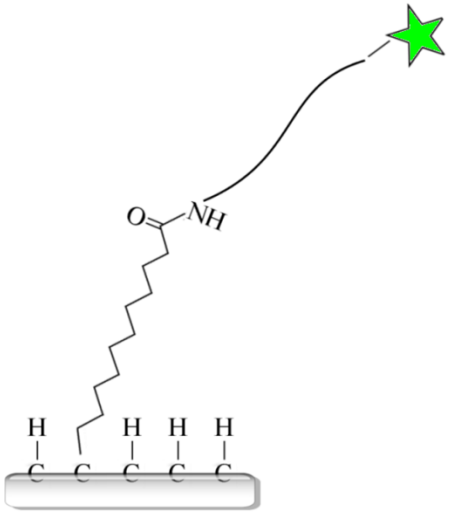
Research question:

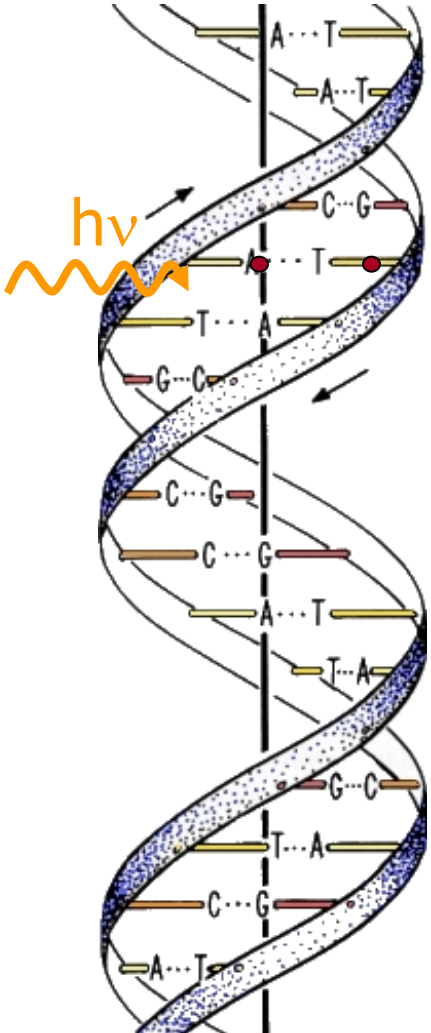
Angle between DNA and diamond?



S. Wenmackers *et al. Langmuir* **24 (2008)** 7269-7277

Ellipsometry of DNA on diamond

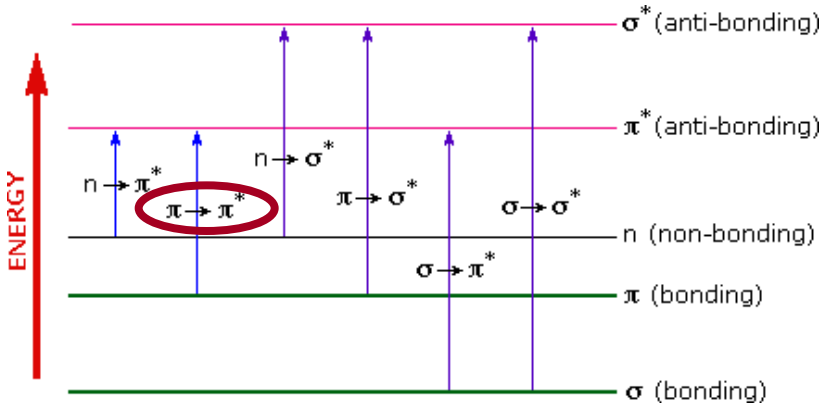
Spectroscopic ellipsometry (UV-Vis)



Bases:

$\pi - \pi^*$ transition

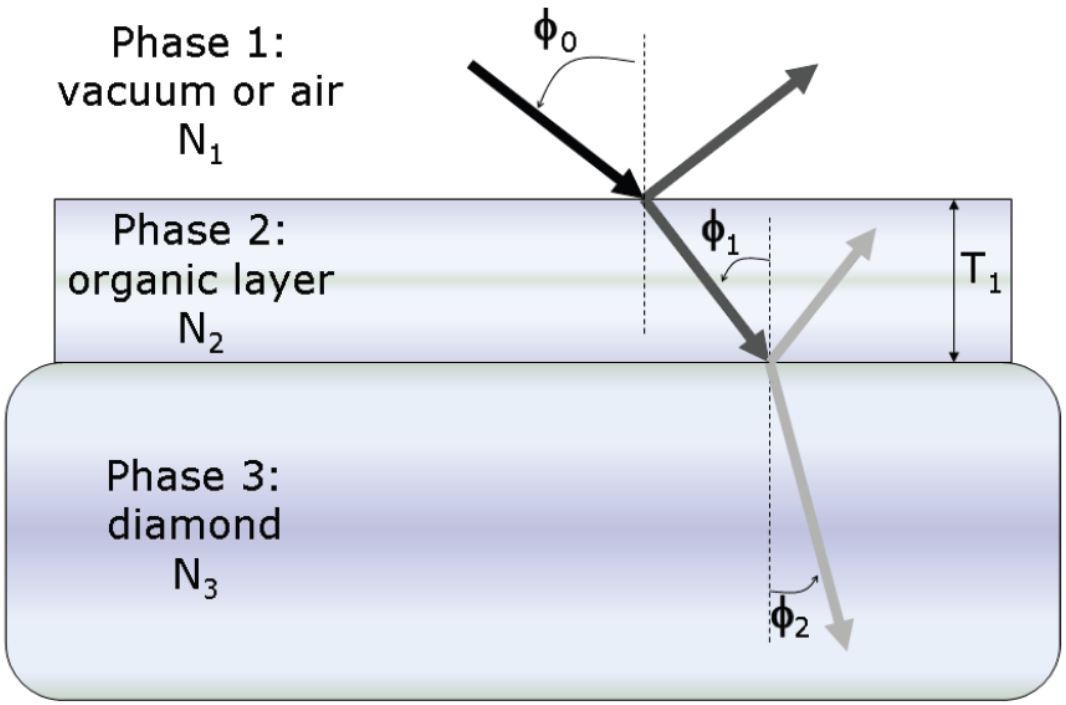
bonding – anti-bonding



Ellipsometry of DNA on diamond

Model:

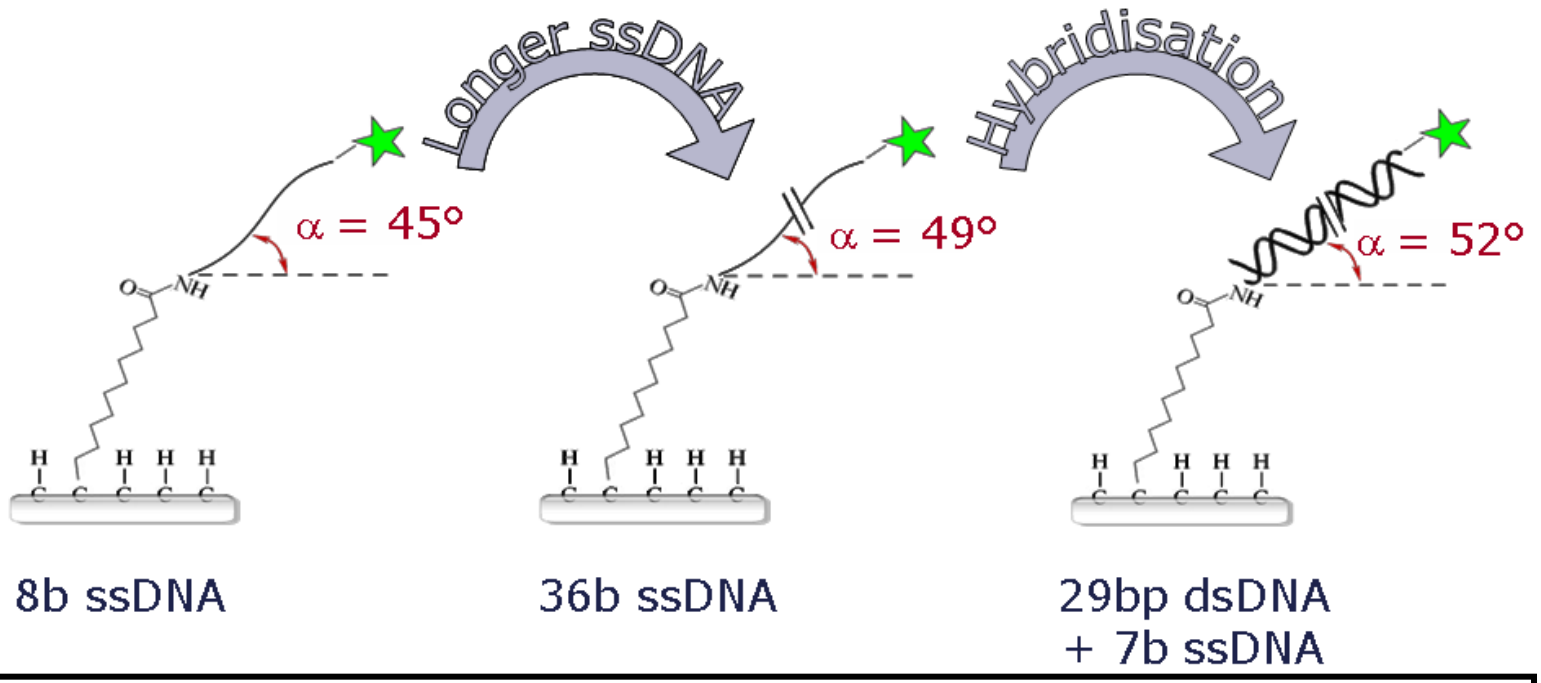
Optical model (three layers)



Ellipsometry of DNA on diamond

Result:

Angle between DNA and diamond



How reliable is the result?

Ellipsometry of DNA on diamond

Traditional view on models:

Model describes a target system,

part of reality

Our target system
= diamond-based DNA sensor
⇒ something that doesn't exist (yet)

In material physics & engineering, target system may be an ideal model.

Ellipsometry of DNA on diamond

Sample = material model,
iconic model
represents surface of typical diamond DNA sensor

Protocol — ideal model of
Execution of protocol

Nanoscience: result not directly observable

Additional characterization methods

On actual sample or parallel sample?

Main characterization method

Ellipsometry of DNA on diamond

Main characterization method

In casu, UV-Vis ellipsometry

Complex apparatus connected to synchrotron

Raw data

↓ **Selection of 'good' spectra**

Clean data = model of the actual data

Ellipsometry of DNA on diamond

Information on experimental method

physical theory (optics), design of apparatus

+ Information on sample

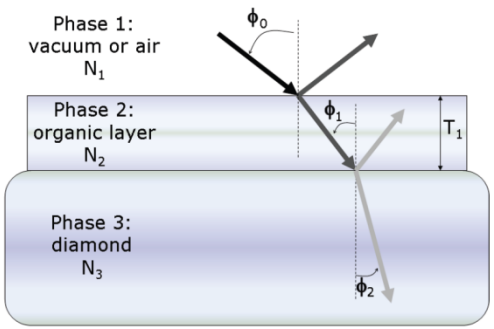
protocol, outcome of additional tests

⇒ Mathematical model

- Additional parameters: only if theory gives them physical interpretation
- Involves idealizations (flat layers) and other approximations

Different representations

Müller matrices,
schematic drawing



Ellipsometry of DNA on diamond

Simulate spectra based on the mathematical model & fit to clean data

Determine α from values of best fit

Conclusions Case 1

☹ **Result is very likely to be wrong**

cf. **Ioannidis PLoS 2005**

☺ **Experiment was repeated: same α**

At least, method is robust $\Rightarrow$
can be used to compare sample parameters

Observe:

Even if we had computed error on α,
it would only inform us of error in fit
= very last step in chain

Case 2
STM of nanowires on Ge(001)

Introduction of case

research question, method, and result

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Analyze experiment & calculation

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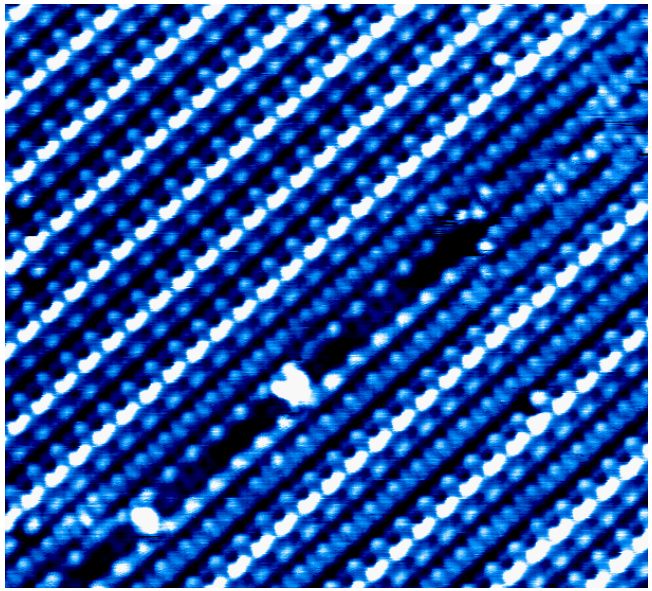
Conclusion

STM of nanowires on Ge(001)

Pt-induced nanowires on Ge(001) observed by STM



Research question:

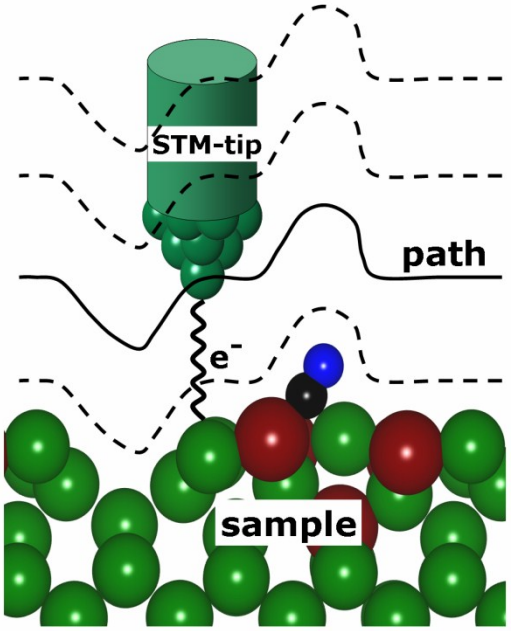
Nature of the wires (Pt, Ge, …)?

D.E.P. Vanpoucke & G. Brocks *Phys. Rev. B* **81 (2010)** 085410

STM of nanowires on Ge(001)

Measurement technique:

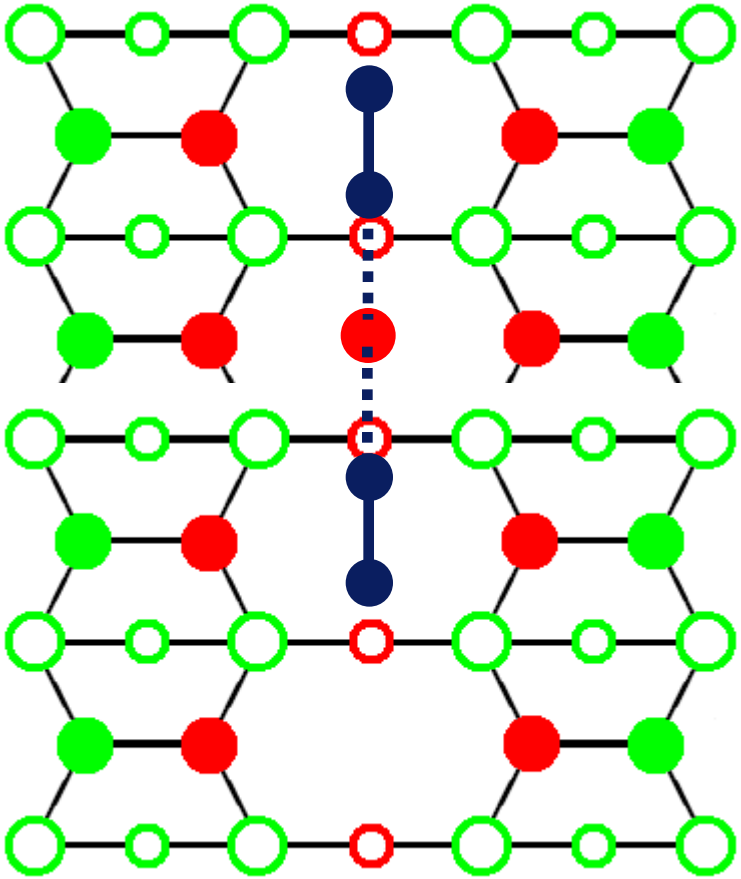
Scanning Tunneling Microscopy (STM)



STM of nanowires on Ge(001)

Model:

Atomistic model



- Pt atoms
- Ge atoms
- Pt or Ge dimer

STM of nanowires on Ge(001)

Result:

The nanowires are made of Ge

How reliable is the result?

STM of nanowires on Ge(001)

Information on experimental method

quantum mechanics (QM), how STM works

+ Information on sample

Protocol (% Pt), preliminary tests

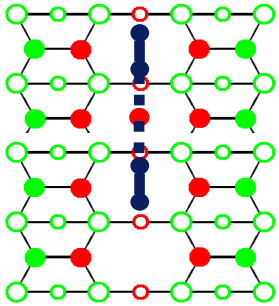
⇒ Atomistic model

Involves approximations

- approx. QM to density function theory (DFT)
- isosurface of charge density = tunneling
- periodic boundary conditions (∞ area)
- 0K, 0Pa, STM-tip = point source

Different representations

list of coordinates,
schematic drawing



STM of nanowires on Ge(001)

Simulated STM images based on various atomistic models.

Compare to experimental images.

Refine atomistic models (combine structures).

No actual fitting occurs:
ab initio (from theory)

Identify best match: underlying model structure of this best-match is taken to be actual structure of the sample

Conclusions Case 2

Strong point of this case:

ab initio, no statistical fitting

The result may still be wrong, *e.g.* if:

- all atomistic models were wrong
  - contamination of sample,
  - different % Pt in actual sample,
  - just not thought of relevant configuration
- some approx. was unwarranted

Atomistic realism:

It is assumed that the atoms are spatially arranged in a specific way = right model

General conclusions

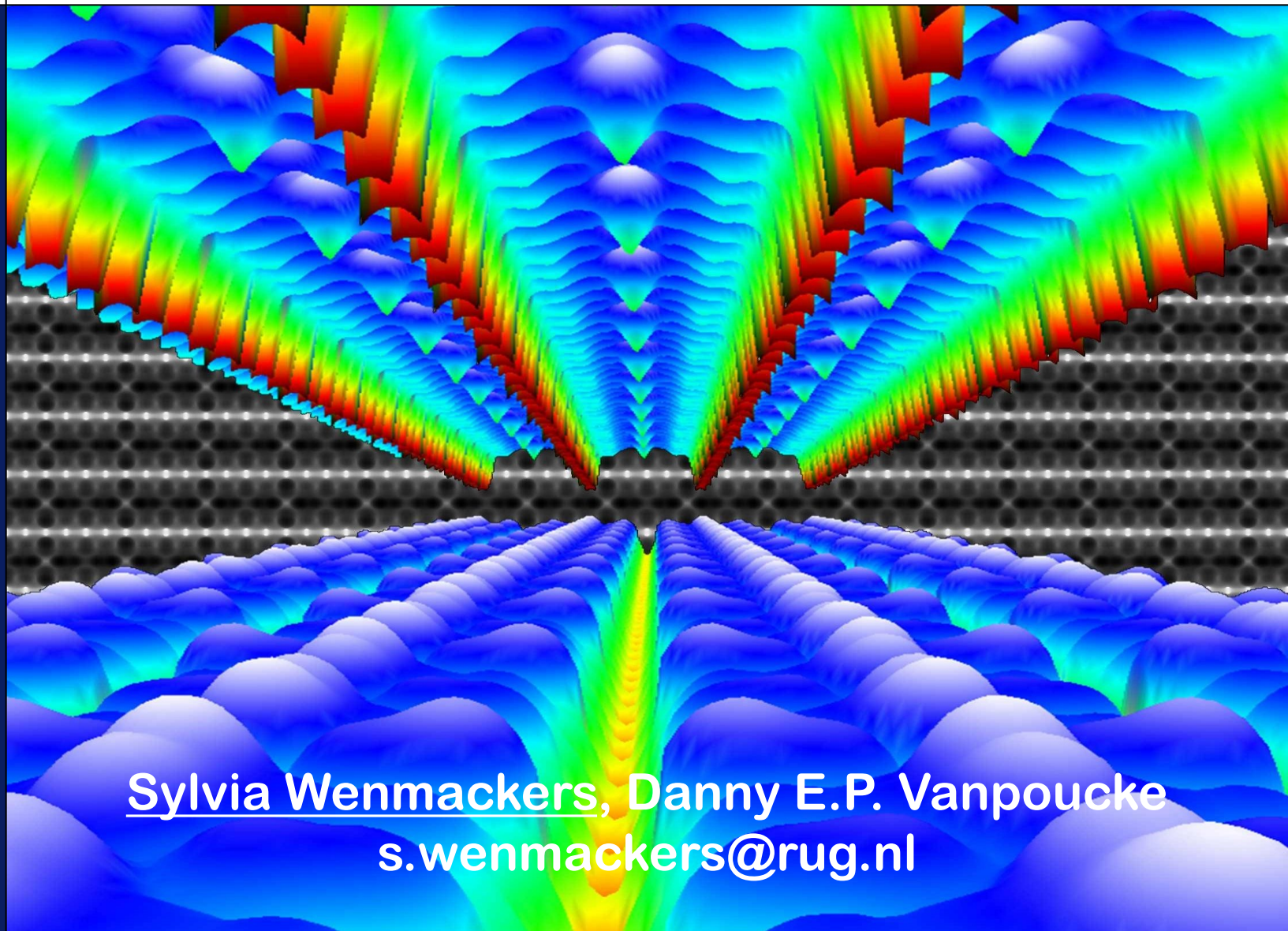
In material science, error bars may provide a false feeling of security

Material scientists tend to be realists about their models

parameters is chosen on the basis of background theory + contextual info rather than some information criterion

university of groningen
faculty of philosophy

Thank you for your attention



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