数理モデリングで未来を創る
～次世代の電気材料へ～

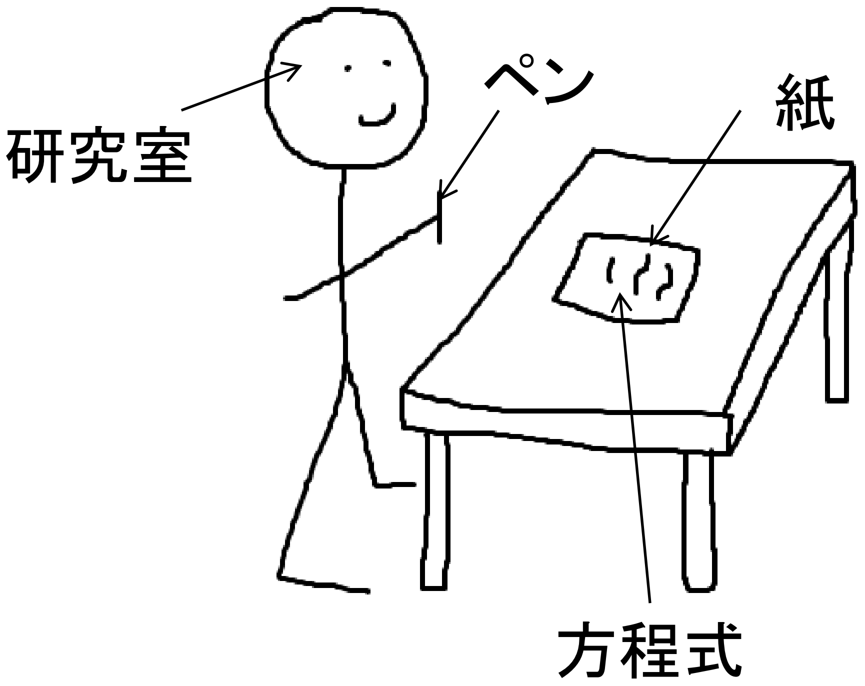
Daniel Packwood　（パックウッド・ダニエル）

東北大学　原子分子材料科学高等研究機構
科学技術振興機構　さきがけ

東北大学

原子分子材料科学高等研究機構
Advanced Institute for Materials Research

さきがけ
PRESTO

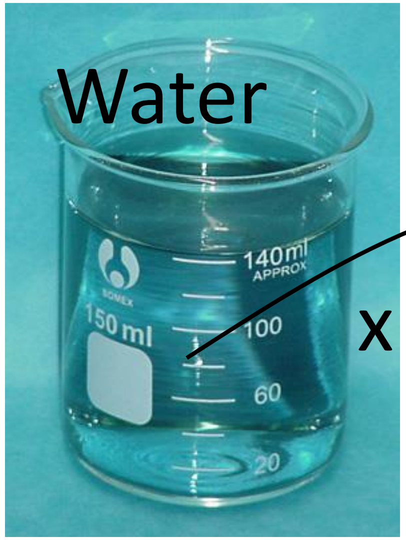


I am a **chemist** and an **applied mathematician.**

Chemistry = Science of creating new materials using molecules

Applied Mathematics = Science of abstracting natural phenomena

Molecules make up matter



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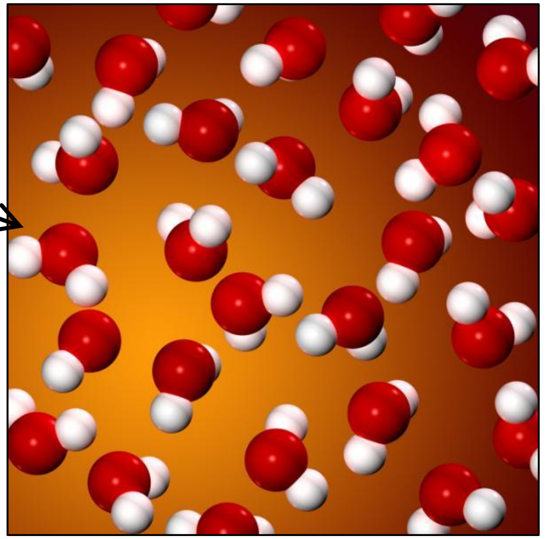
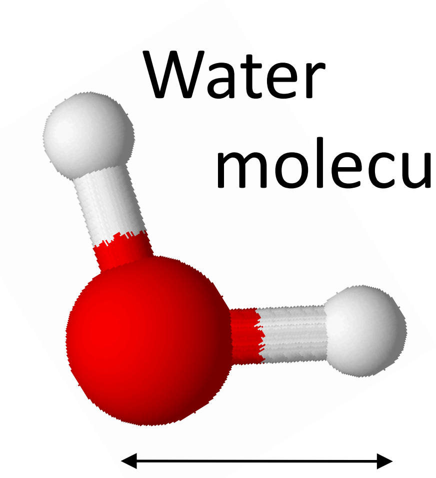




Water molecule

9.6 x 10^{-9} cm

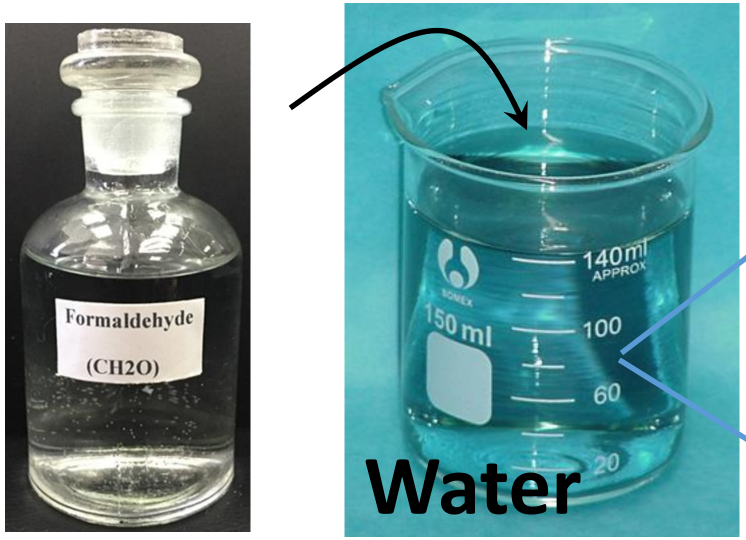
(0.0000000096 cm)

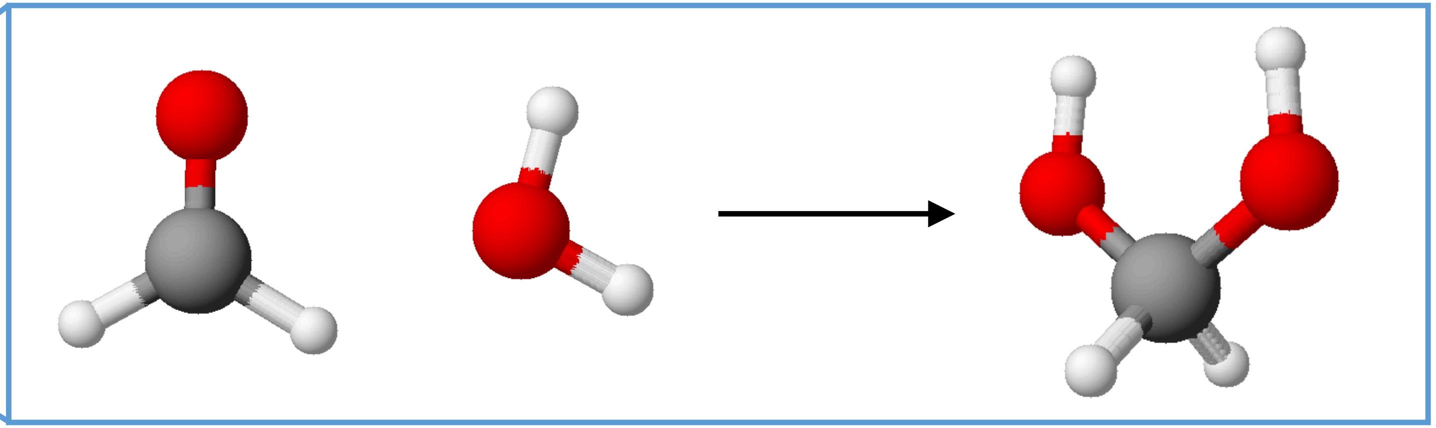
How to make new materials using molecules?

1. Chemists mix molecules together.

2. Molecules **interact** with each other

3. **Sometimes, interaction produces new material**





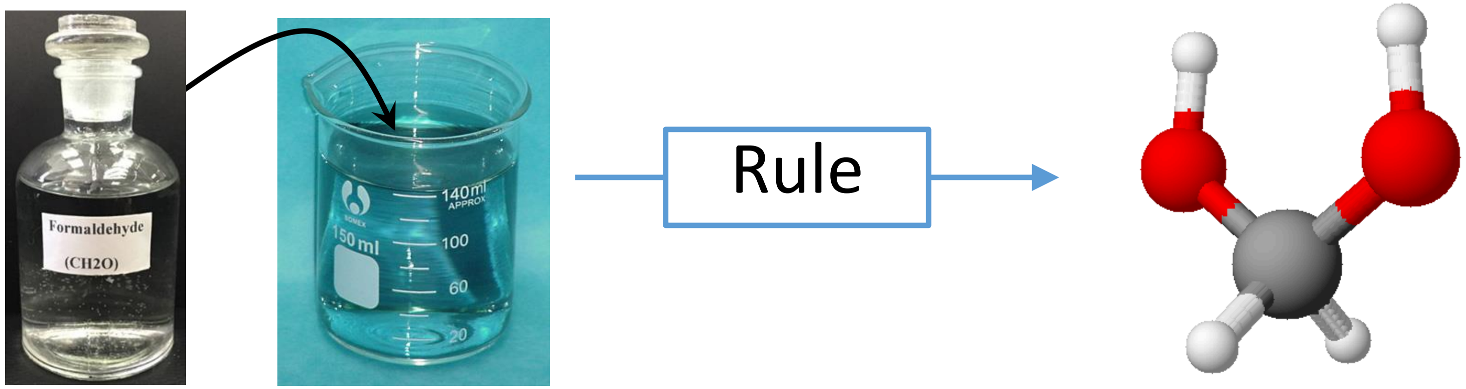
Chemists **can control this step**

Chemists **cannot control** this step!

Key point: Before mixing the molecules together, chemists must **know the rules** for how the molecules will interact.

What is a rule?

A ‘rule’ predicts what happens ***without* doing an experiment.**



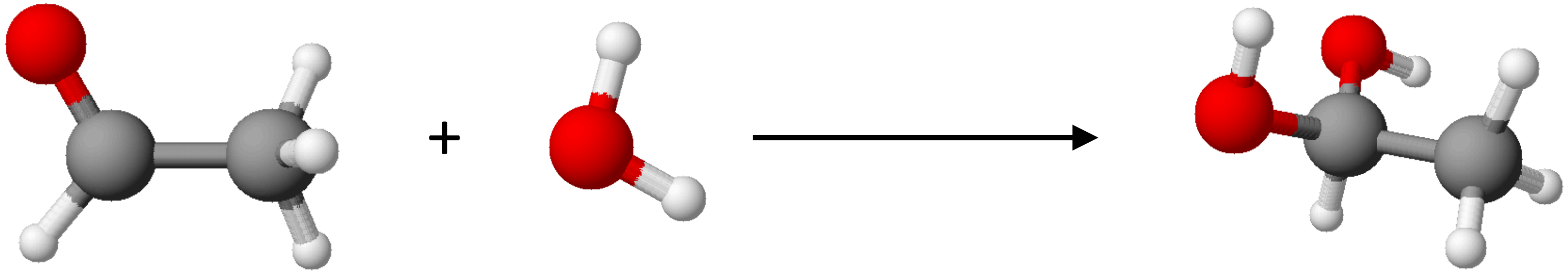
How to deduce new rules?

This is very difficult.

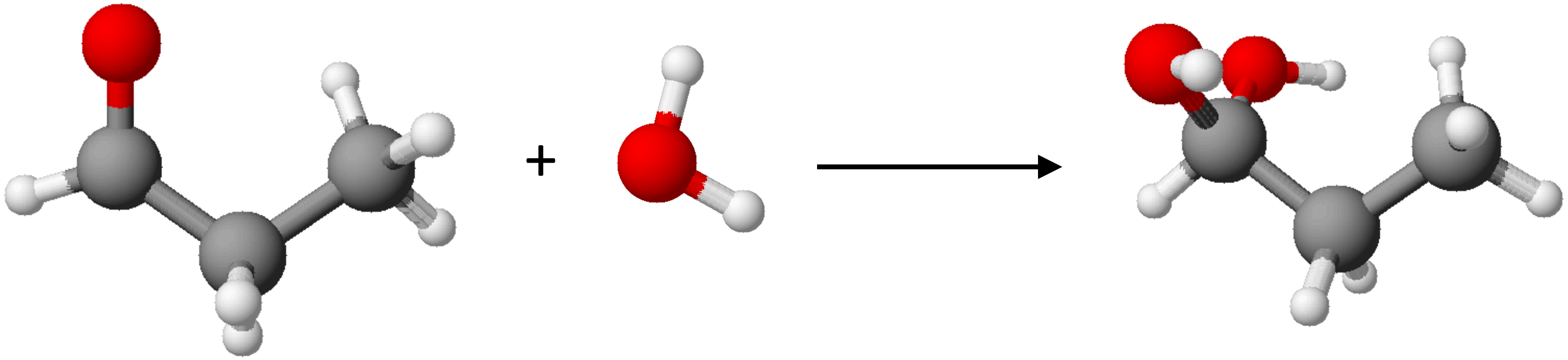
A chemist needs to do **many, many experiments**…

Example: Let's deduce a rule!

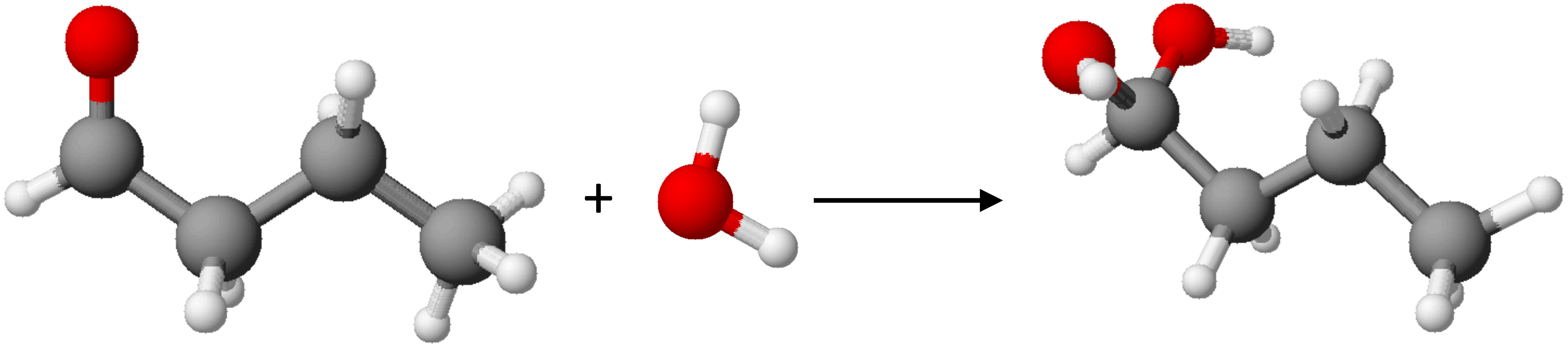
Experiment 1



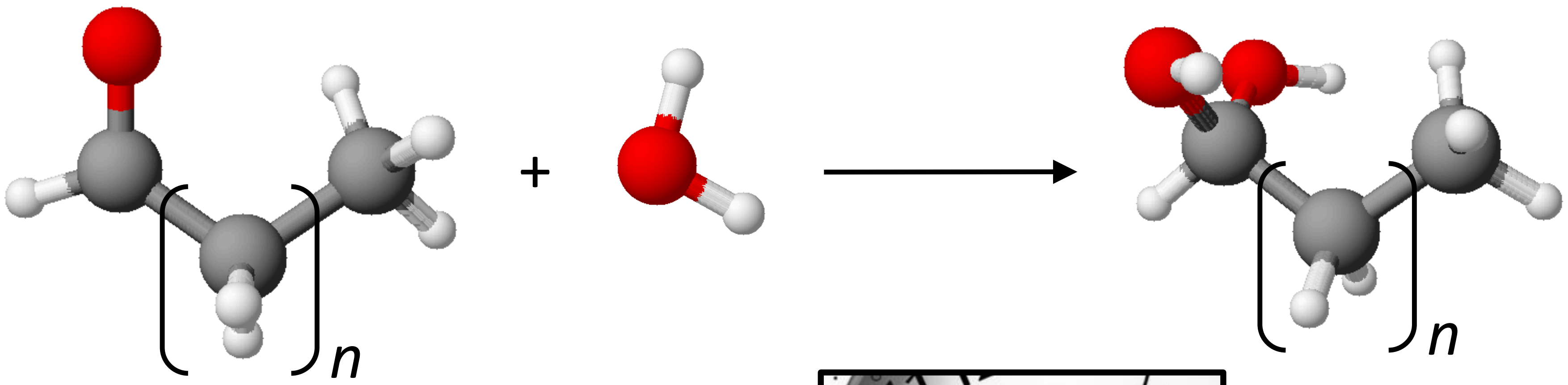
Experiment 2



Experiment 3



Rule ($n \geq 1$)



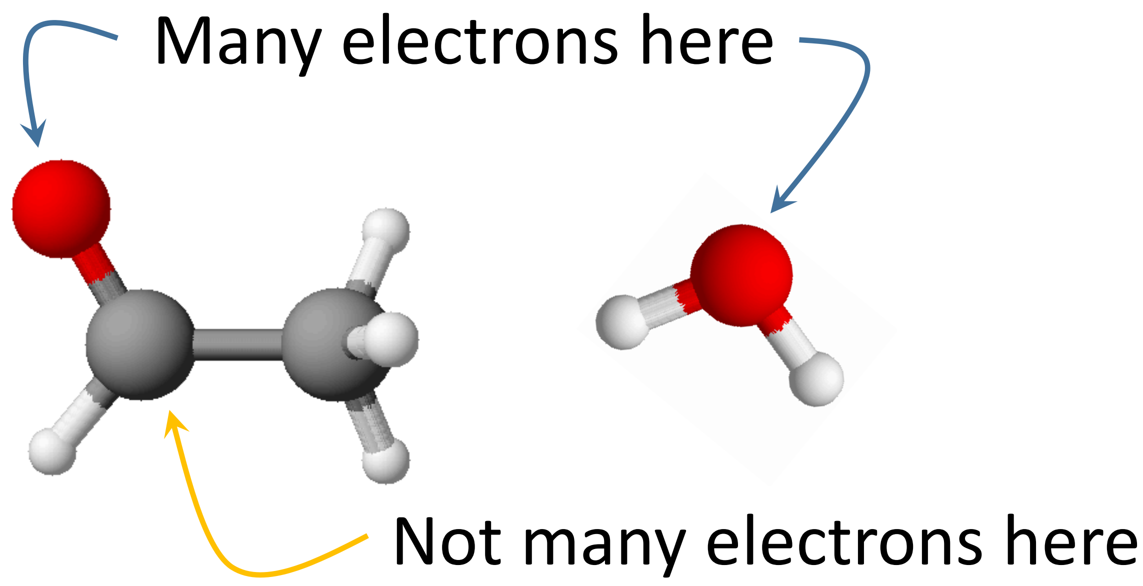
Why is it hard to deduce rules?

Chemist must do **many, many experiments.**

- Experiments take a **long time**.
- Experiments are often **dangerous.**
- Experiments cost **a lot of money**.

But there is **another way** to deduce rules… **mathematical modelling!**

Mathematical Modeling Process

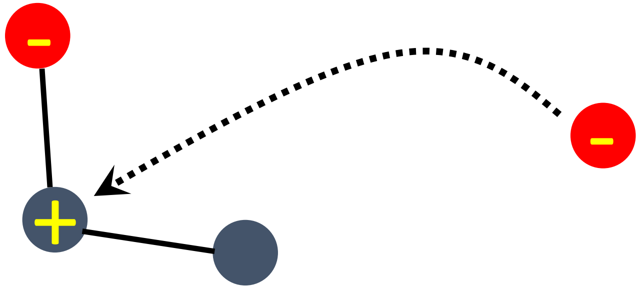


1. Identify the **key parts** of the real situation:

2. **Abstract** the real situation

3. Apply the **laws of physics**

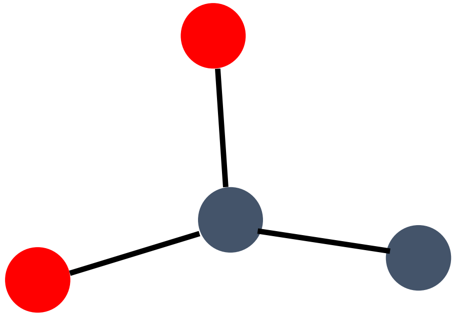
→ Tells us the rule



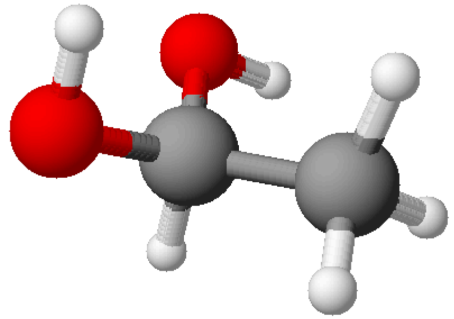
Physics: Positive attracts negative.

4. Compare to **experiment**

Similar → Rule seems reasonable.



Experiment

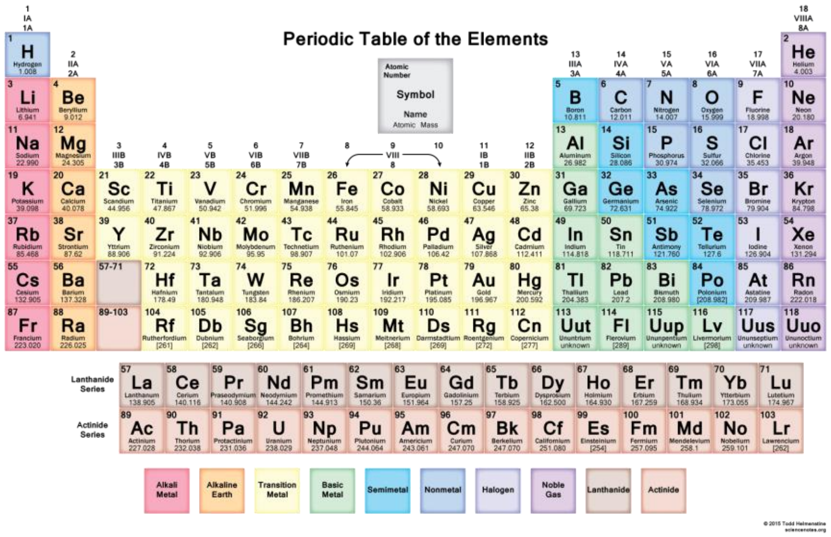


Key Steps for Mathematical Modeling

1. Identify the key parts of the real situation

2. Abstract the real situation

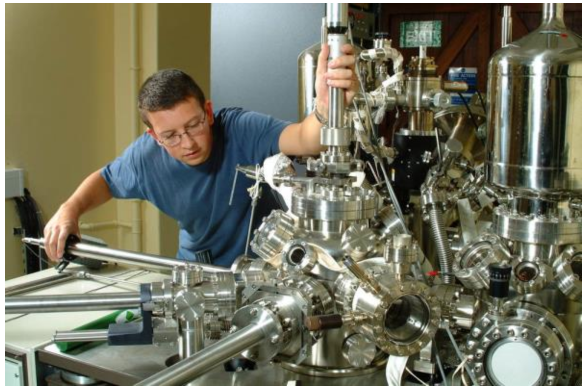
Need a good knowledge of the situation!



3. Apply the laws of physics ← Need to be good at mathematics!

$$\frac{dX_t}{dt} = f(X_t) + b\frac{dW_t}{dt}$$

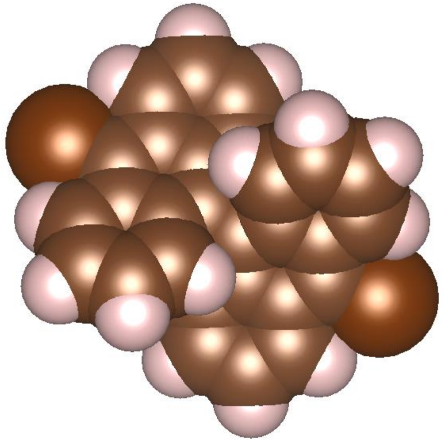
4. Compare to experiment ← Need friends who can do experiments!



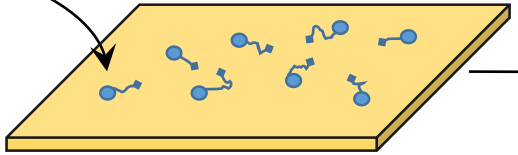
Mathematical modelling for next-generation electrical materials

Experiment by P. Han, T. Hitosugi (2014, Tohoku University)

Di-bromo bi-anthryl (DBBA) molecule

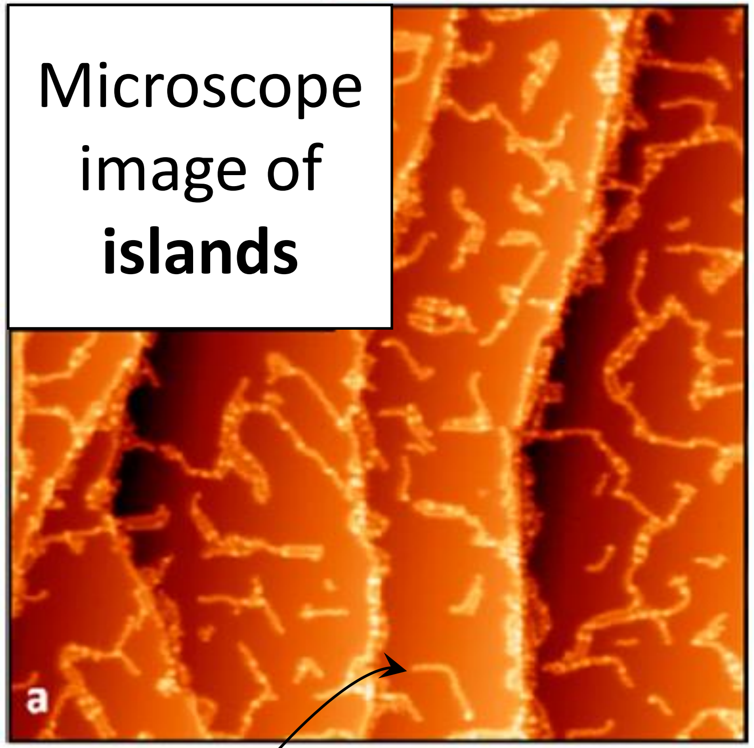


Place on copper surface



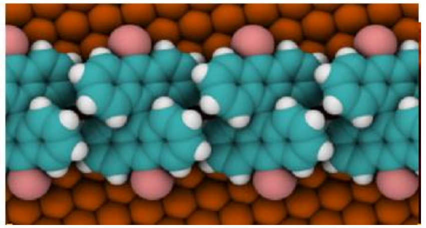
Molecules diffuse on surface

1.380 x 10^{-7}m



1.380 x 10^{-7}m

'Molecule island'

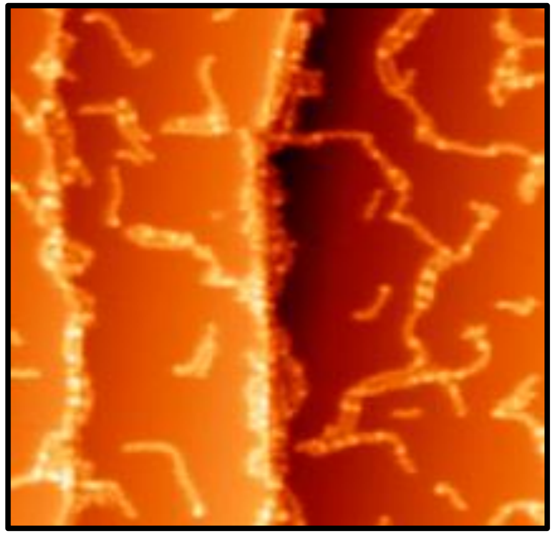


What happened?

The molecules **assembled into islands**.

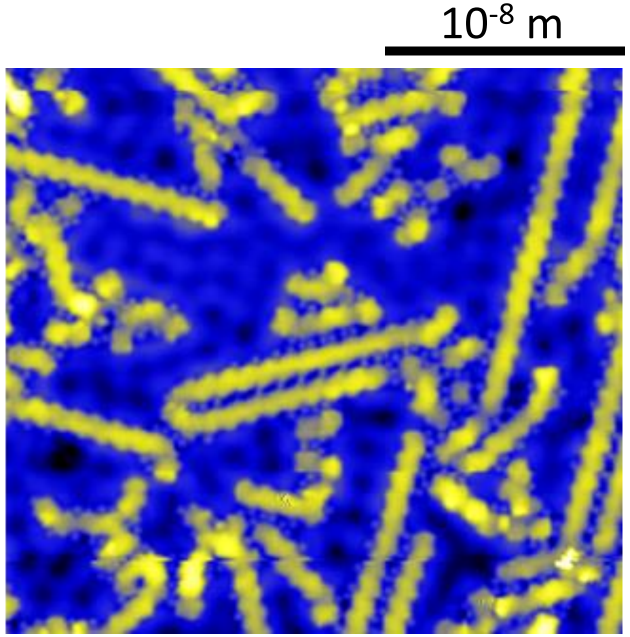
This phenomenon is called **molecular self-assembly.**

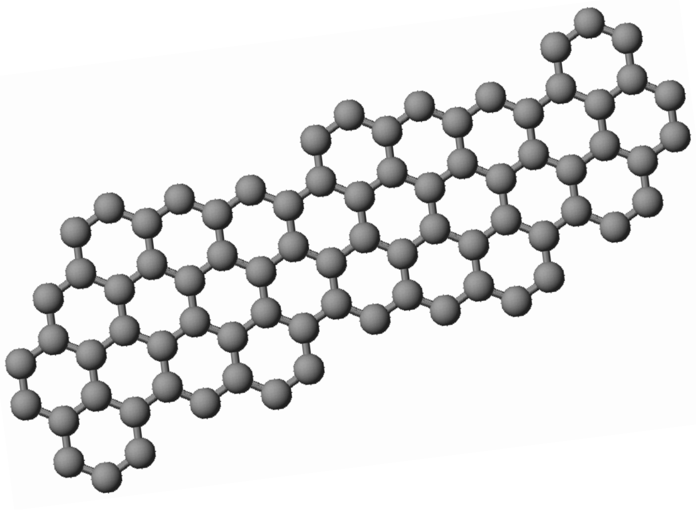
Molecular self-assembly is **very useful**…



Heat

(800 ^{o}C)





Islands turn into **graphene**

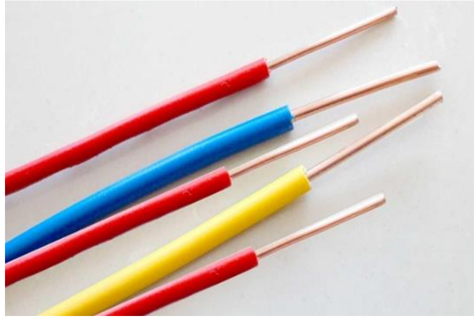
What is special about graphene?

Graphene has **extremely high conductivity** (more than 2000 x silicon)

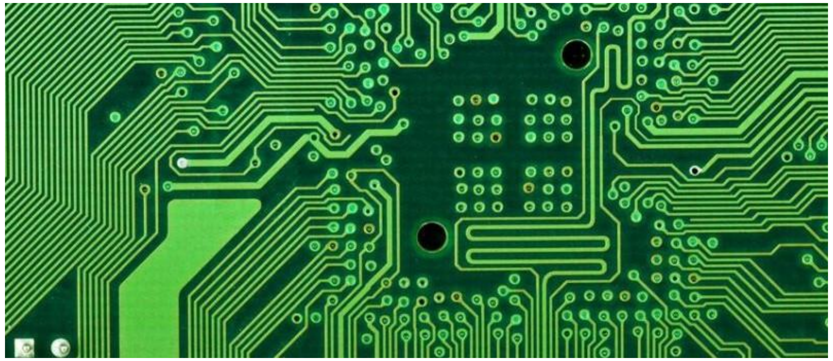
Dream: Create **real electronics** using graphene (e.g., extremely fast computers).

How might we make real electronics using graphene?

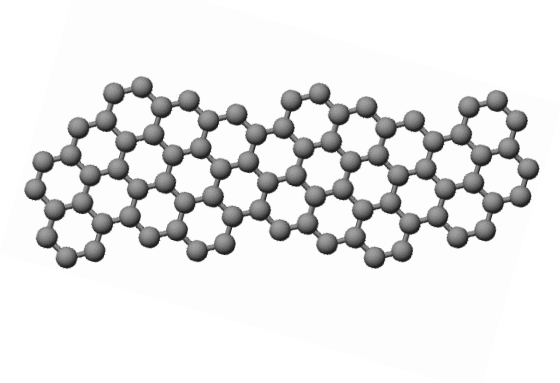
Wire:



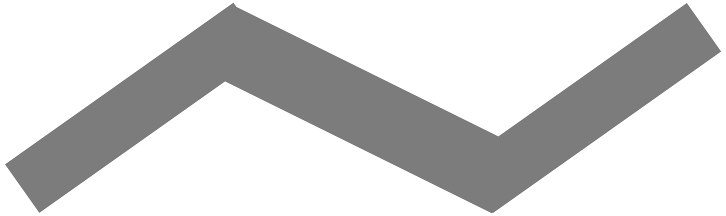
Electronic circuit:

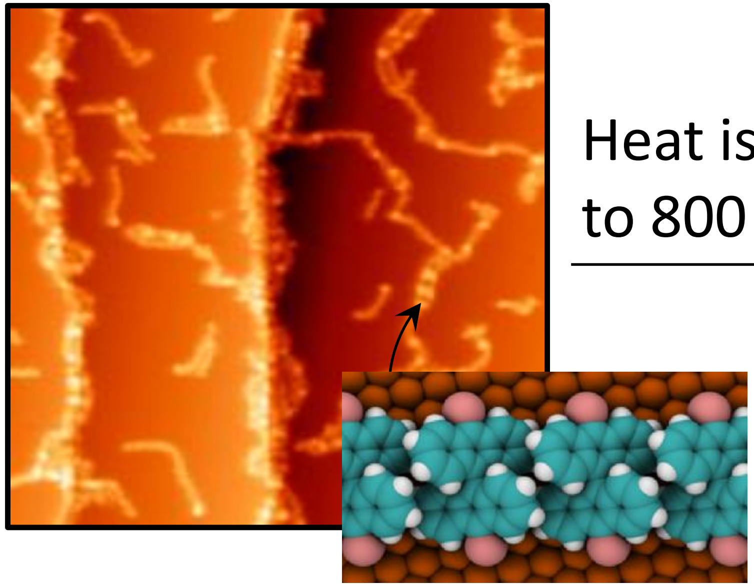


Wire-shaped graphene



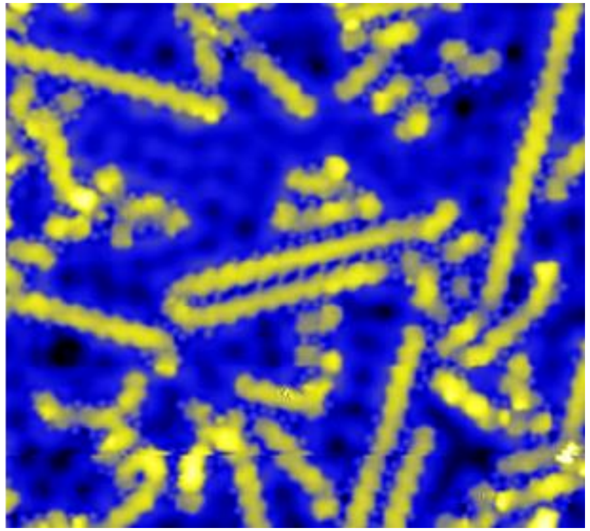
Non-straight wires





Wire-shaped island

Heat islands to 800 ^{o}C →



Wire-shaped graphene

How to make?

Control island structure

→ Control graphene

But, **nobody knows the rules** for island formation.

Let's try mathematical modeling!

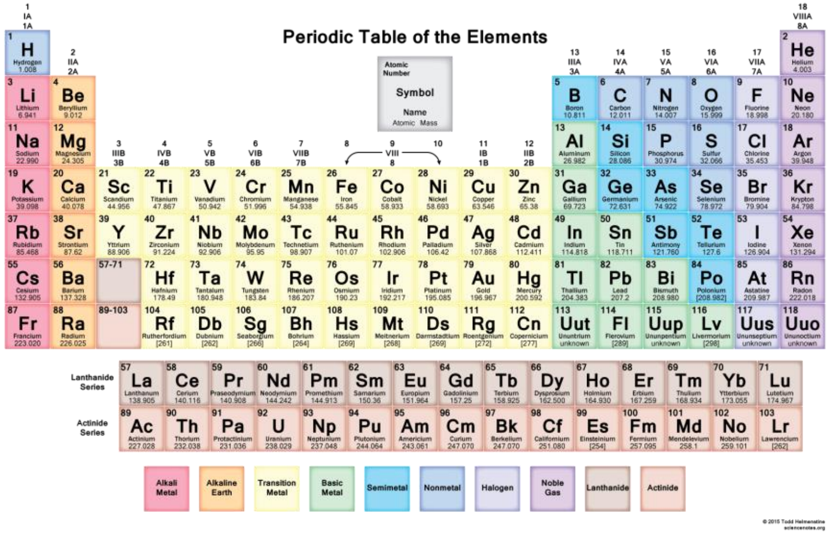
Mathematical modeling for island formation

1. Identify the key parts of the real situation.

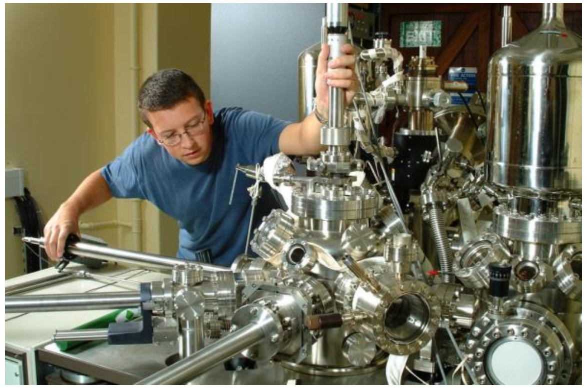
2. Abstract the real situation

3. Apply the laws of physics

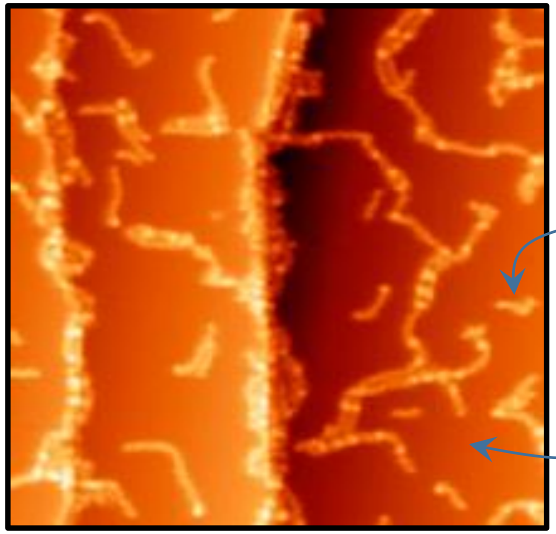
4. Compare to experiment



$$\frac{dX_t}{dt} = f\left(X_t\right) + b\frac{dW_t}{dt}$$

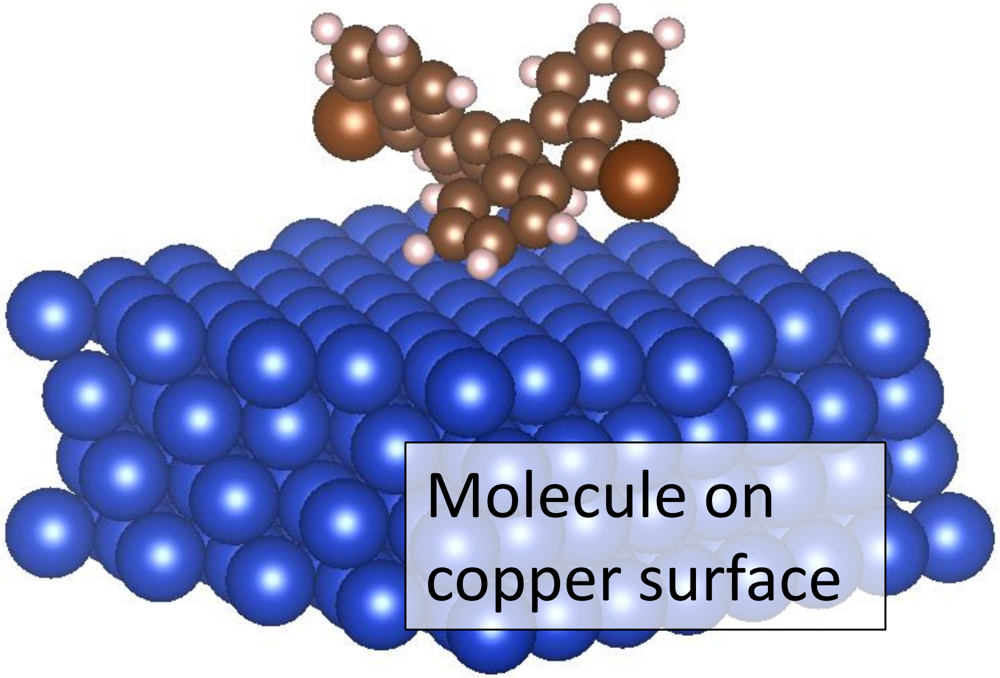


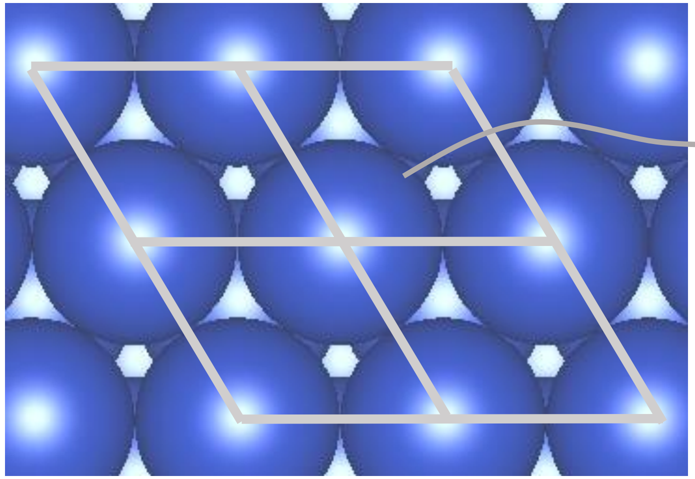
1. Key parts of the real situation



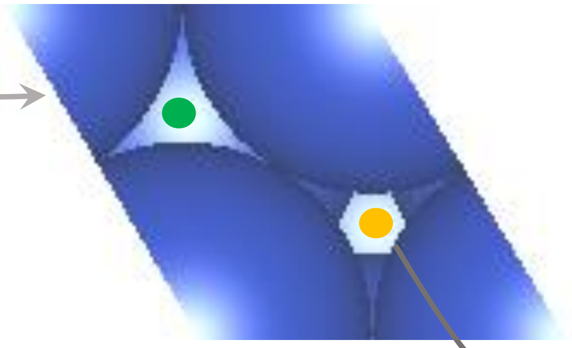
Island made of molecules

Copper surface

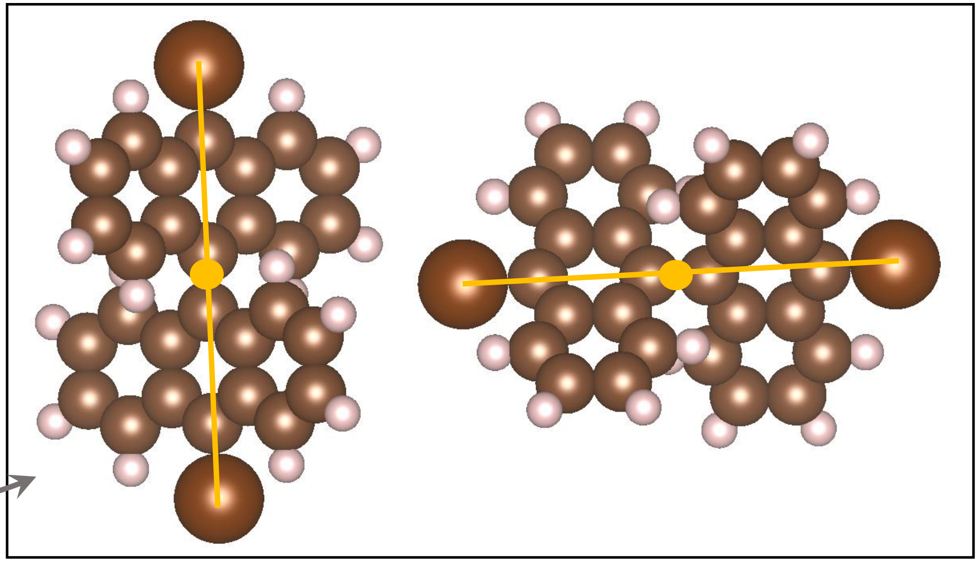




Unit cells of
metal surface

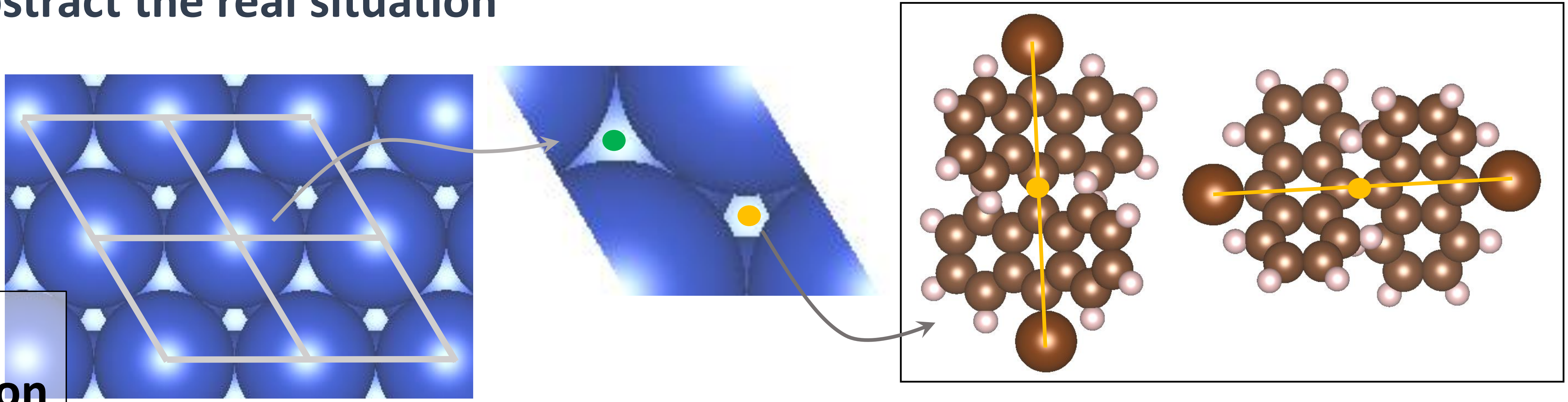


Adsorption sites



Molecule orientations

2. Abstract the real situation

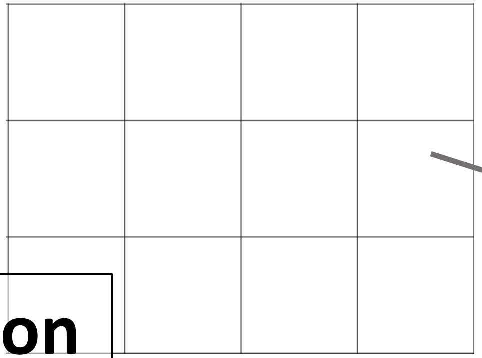


Real situation

Unit cells of metal surface

Adsorption sites

Molecule orientations



Abstraction

'Cells' $C_1, C_2, \ldots, C_M$

$\left\{ \sigma_1 \quad \sigma_2 \right\}$

'Colours'

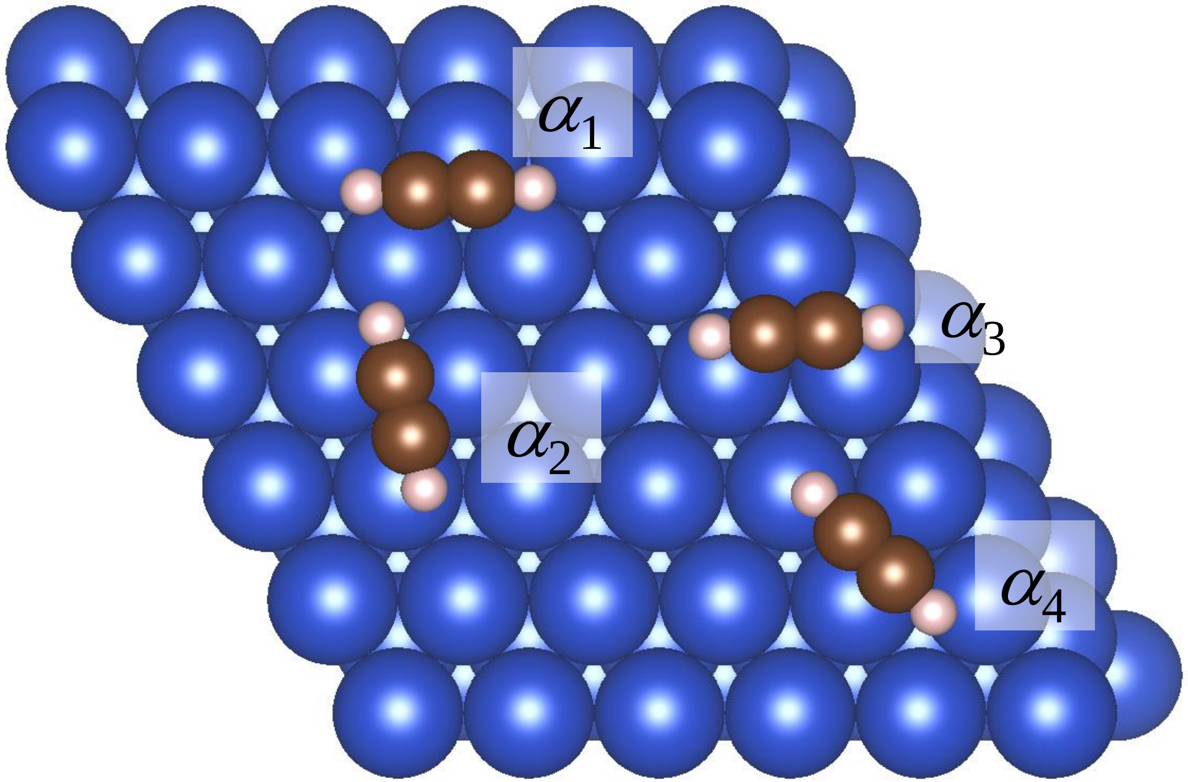
$\sigma_1, \sigma_2, \ldots, \sigma_k$

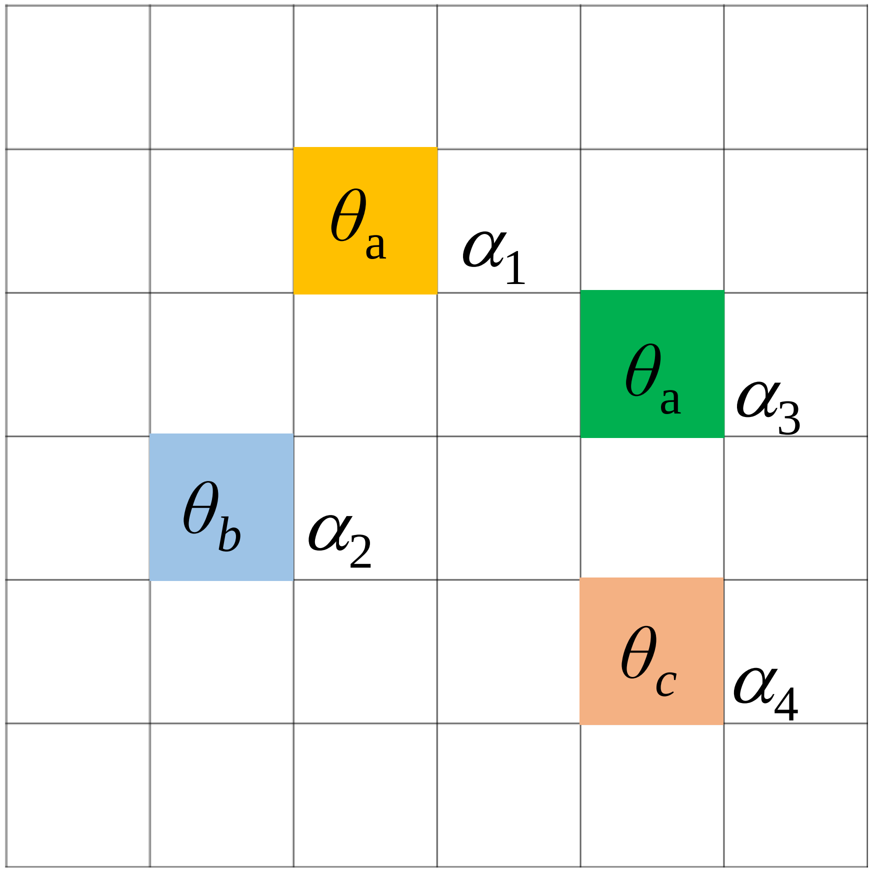
$\left\{ \theta_{2,1}, \theta_{2,2} \right\}$

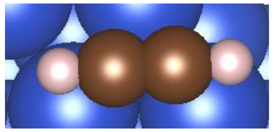
'Shades'

$\theta_{i,1}, \theta_{i,2}, \ldots, \theta_{i,n(i)}$

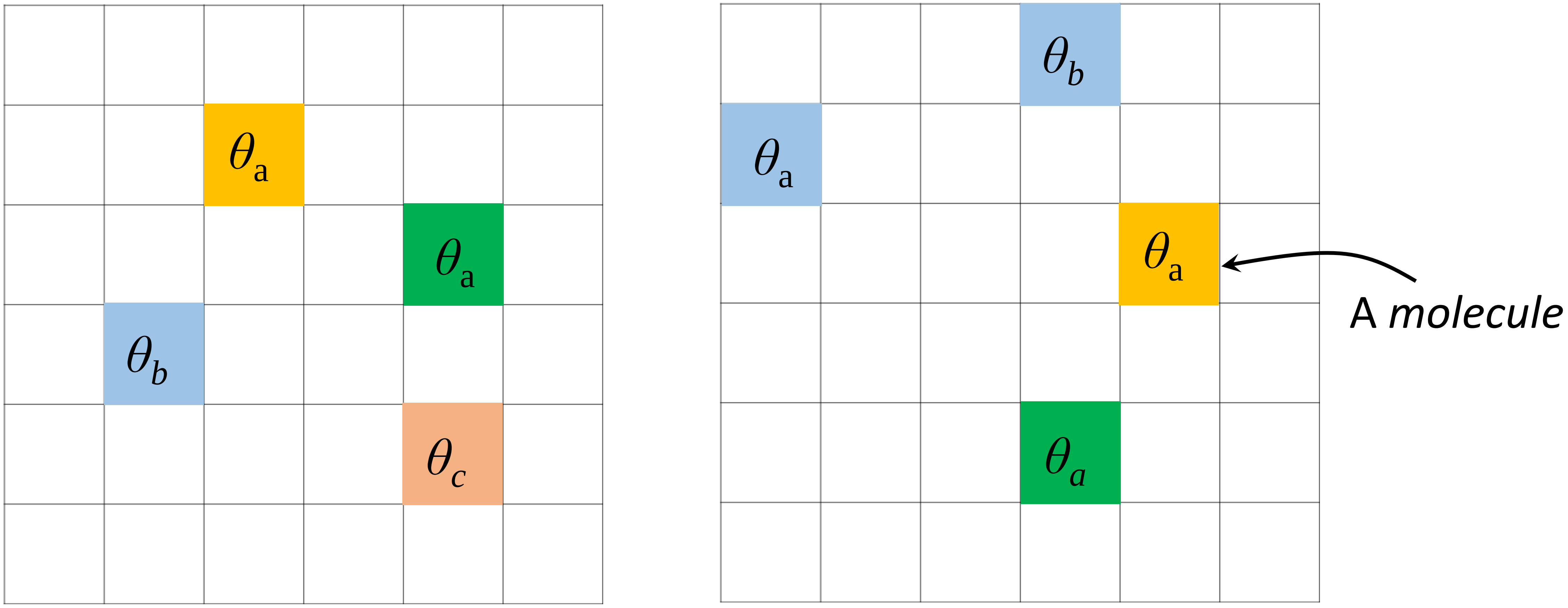
Reality – abstraction correspondence





 = HCCH molecule

A *configuration* is any choice of *N* cells, colours, and directions



Two configurations (*N* = 4, four colors ● ● ● ●, three shades θ_a, θ_b, θ_c)

Mathematical modeling for island formation

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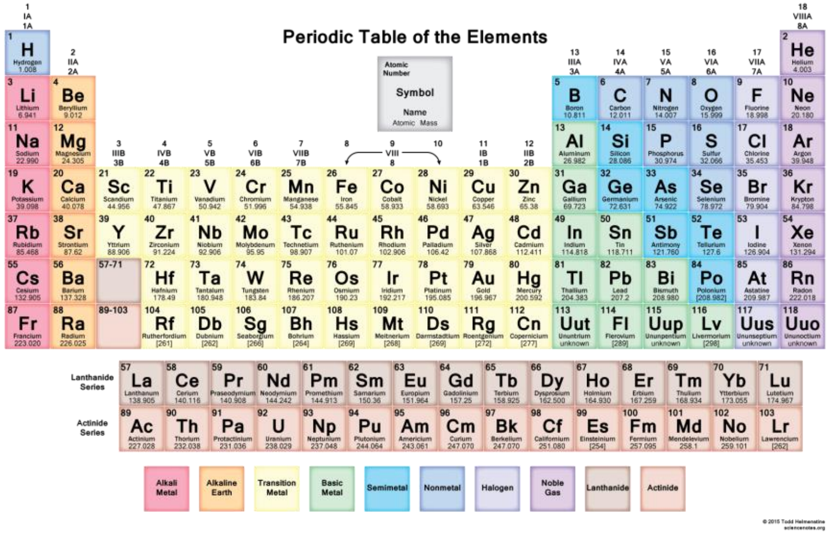
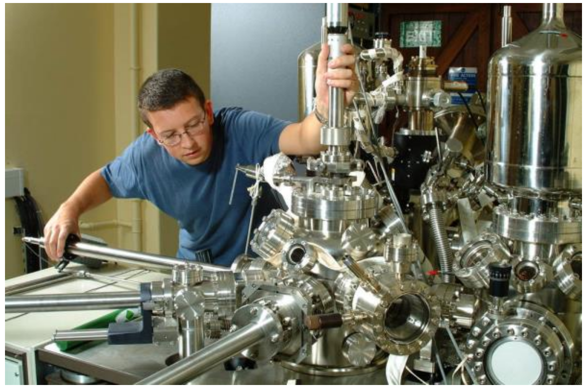
✓ 2. Abstract the real situation

3. Apply the laws of physics

4. Compare to experiment



$$\frac{dX_t}{dt} = f(X_t) + b\frac{dW_t}{dt}$$



Let *c* be a configuration.

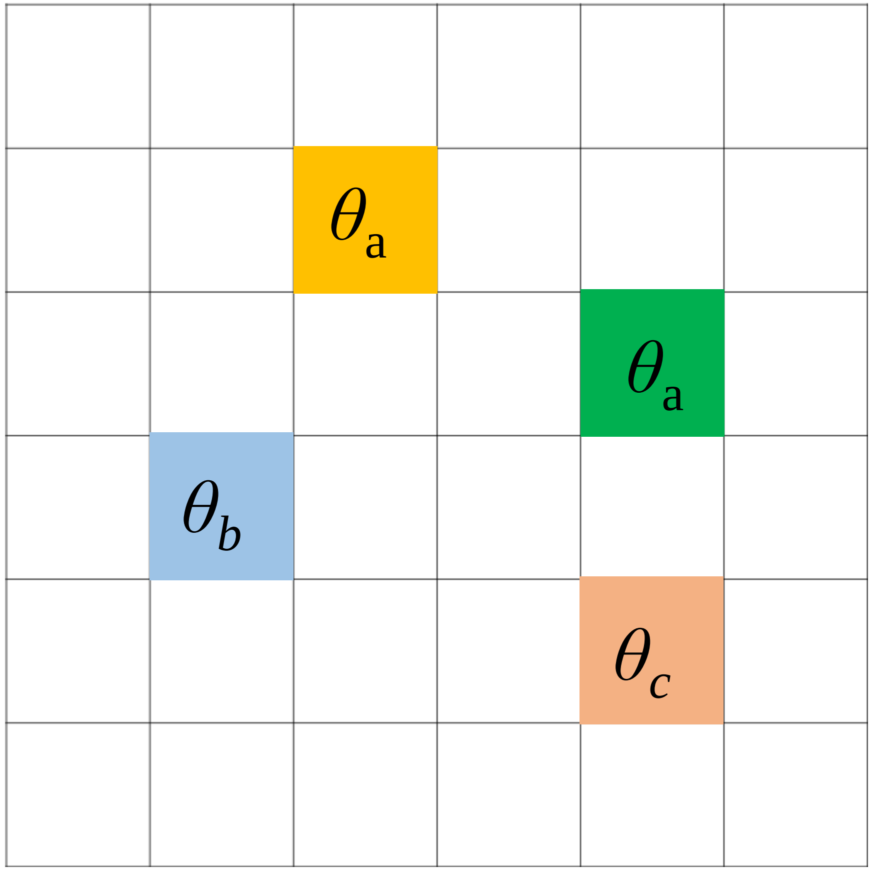
Boltzmann distribution law from physics
→ probability of configuration *c*

$$p(c) \propto \exp\left(-\varepsilon(c)/k_B T\right)$$

$\varepsilon(c)$ = energy of configuration *c* (we can calculate)

k_B = Boltzmann constant (1.38 x 10^{-23} J K^{-1})

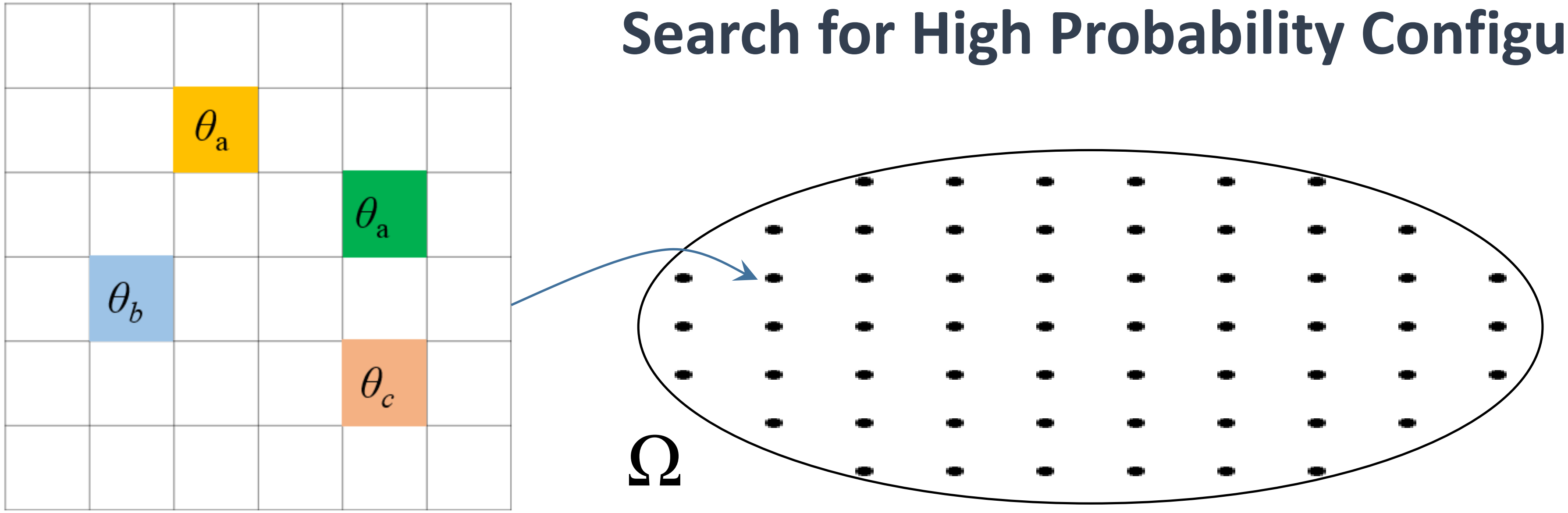
T = Temperature



one configuration (*c*)

Mathematical challenge Find configurations that have high probability.

Search for High Probability Configurations



Ω = configuration space

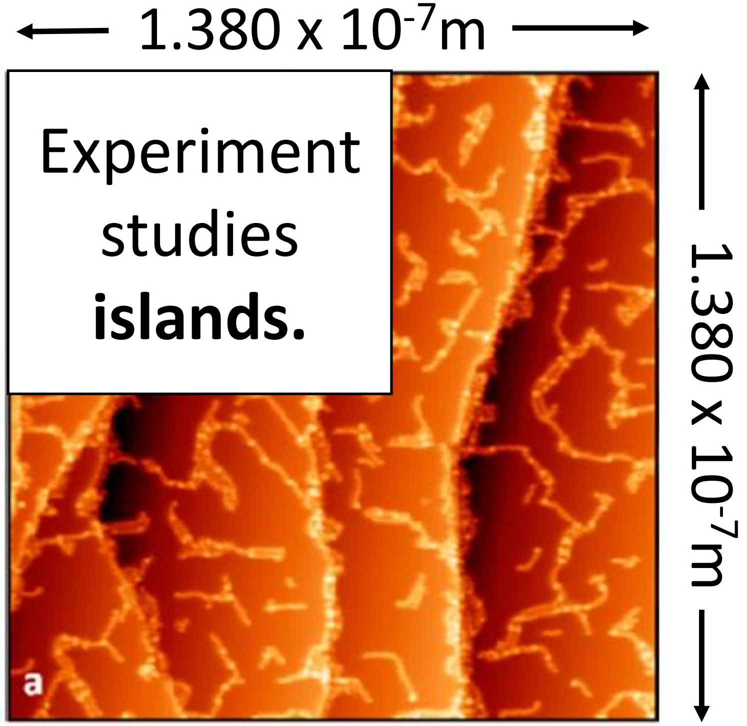
Configuration space is extremely big!

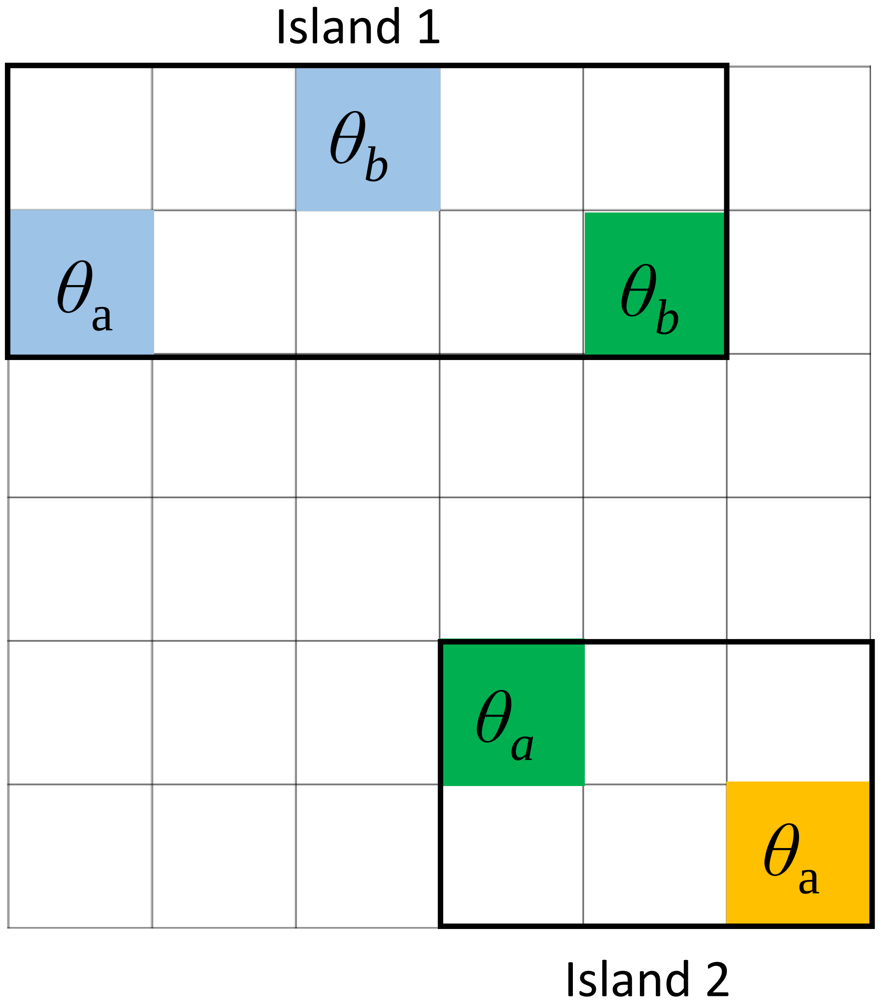
Around 10^{23} configurations (case of 1000 cells with 10 molecules)

Suppose it takes 10^{-6} s for computer to calculate probability of one configuration.

Then 10^{23} x 10^{-6} s ≈ 10^{10} years to check probability for every configuration!

With mathematical thinking, a faster approach is possible…

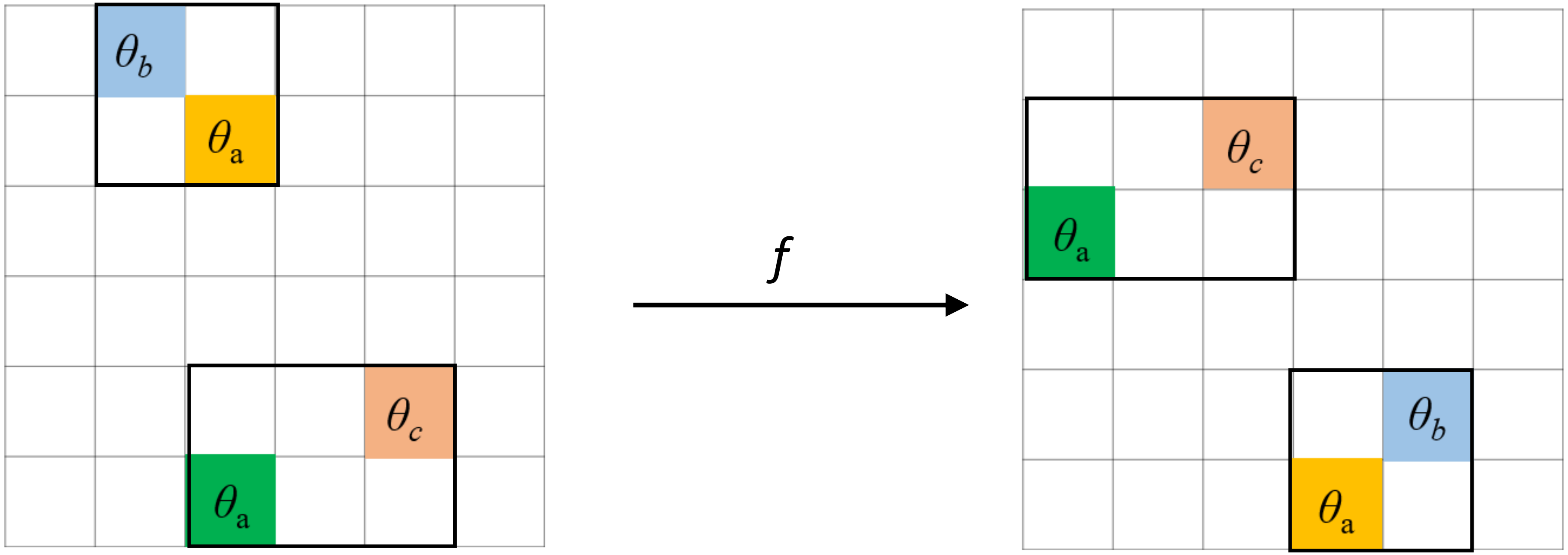




Mathematical definition of **islands?**

An *island* is a group of molecules separated by at least *d* cells.

d is an integer (*d* = 3 in the picture)



Configuration a

Configuration b

Configurations *a* and *b* are different.

But if we

i. rotate the islands of *a*, and

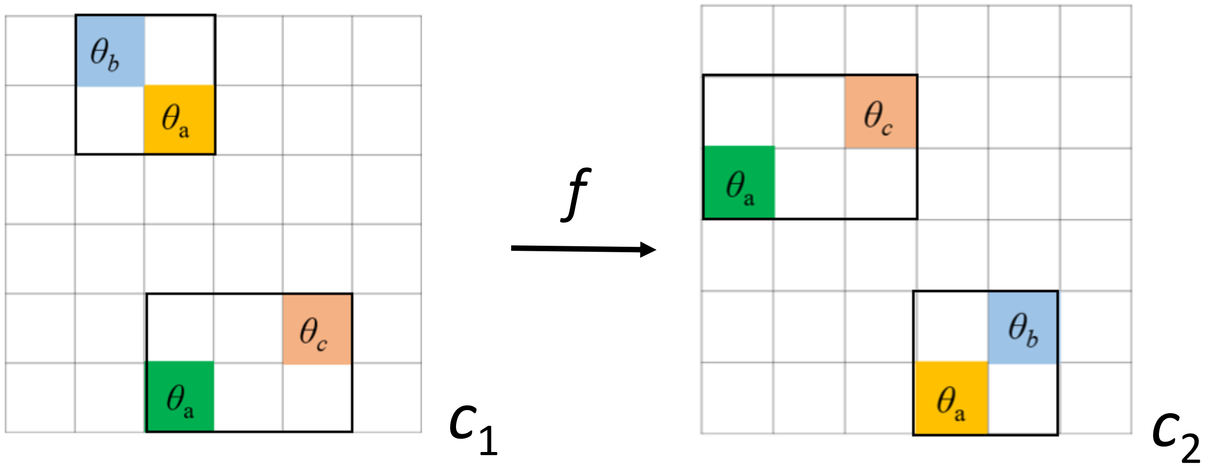
ii. move the islands of *a*,

} f

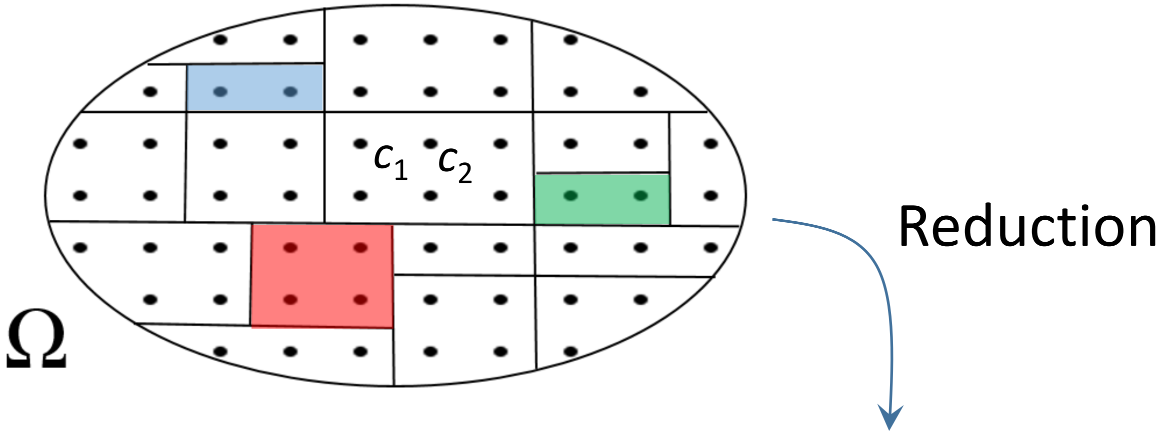
we obtain configuration *b*. So configuration *a* and *b* contain the **same islands.**

Space Reduction

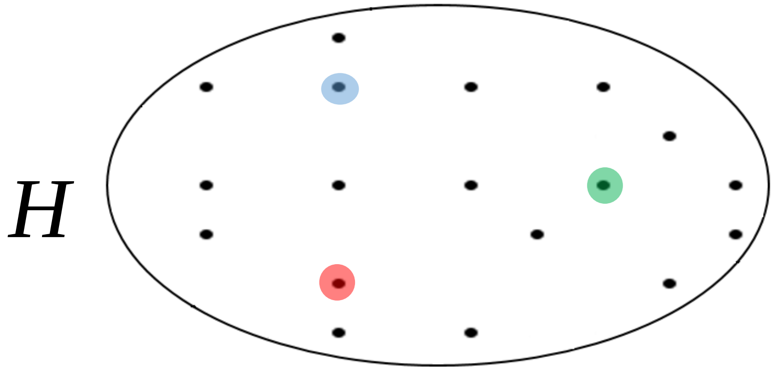
The transformation *f* is called an **isomorphism.**



The isomorphism divides the configuration space into **equivalence classes**



Reduced space H
= collection of equivalence classes



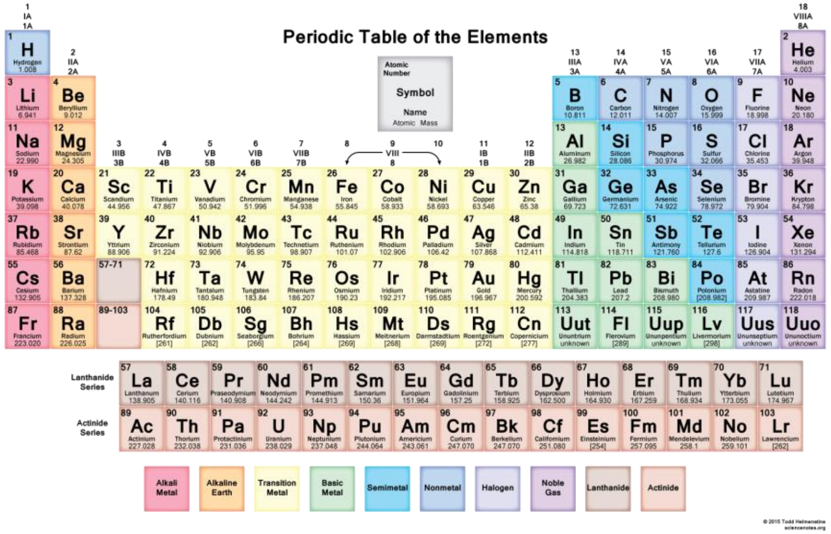
H has around 10^5 elements (10 molecule case)

(compare: Ω has around 10^{23} elements!)

Time to check all probabilities ≈ $10^5 \times 10^{-6}$ s ≈ 0.1s

Mathematical modeling for island formation

✓ 1. Identify the key parts of the real situation.



✓ 2. Abstract the real situation

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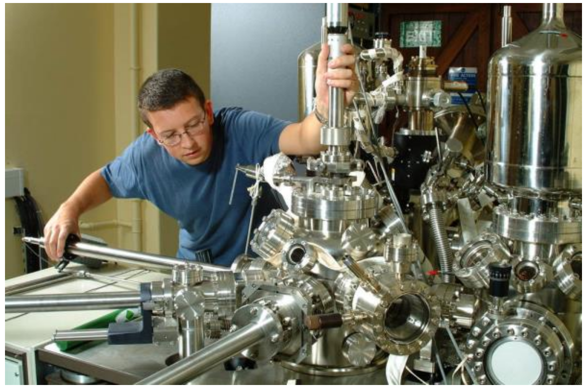
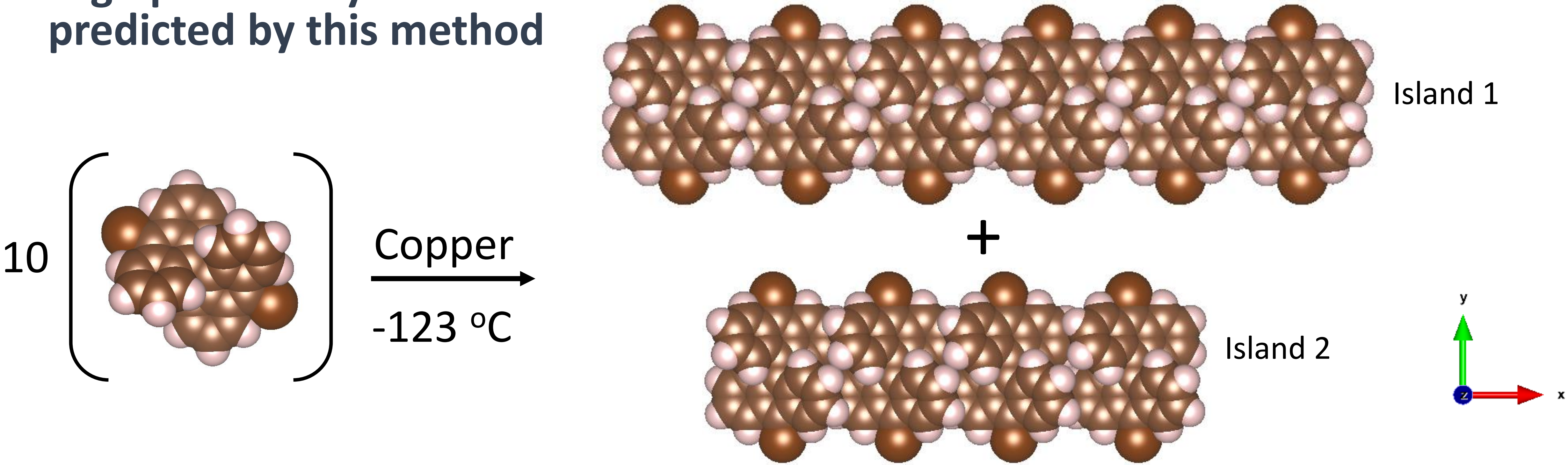
$$\frac{dX_t}{dt} = f(X_t) + b\frac{dW_t}{dt}$$

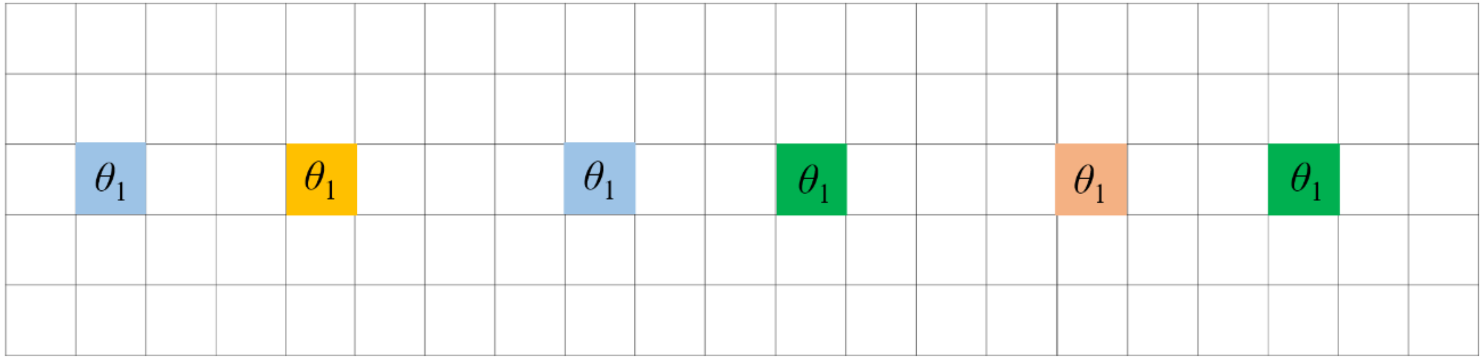
4. Compare to experiment



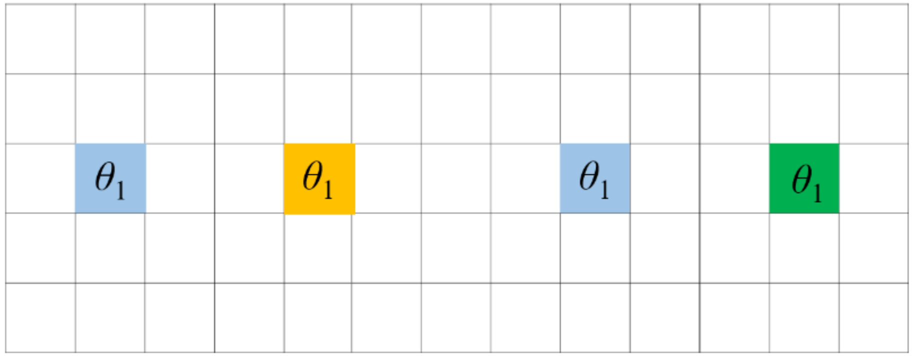
High probability islands predicted by this method



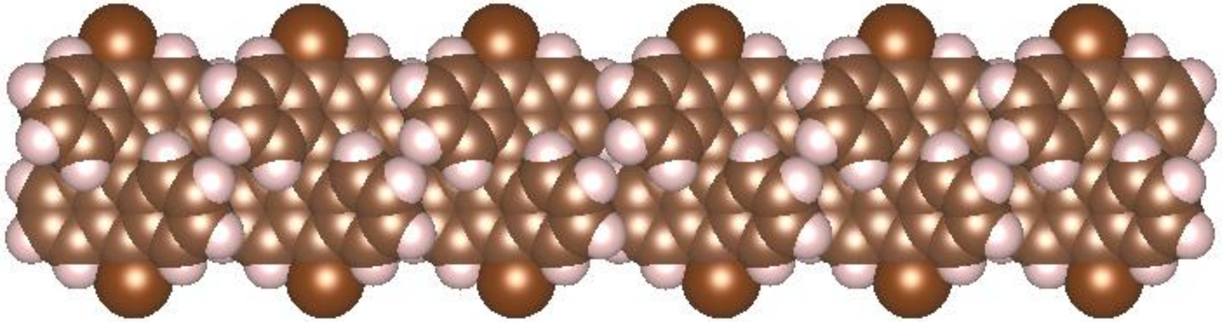
Island 1



Island 2

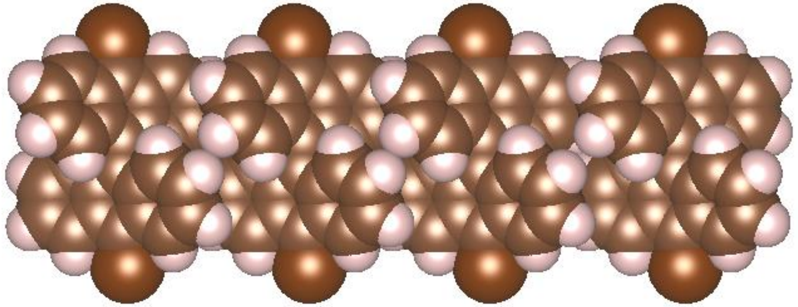


Mathematical modelling (-123ºC)



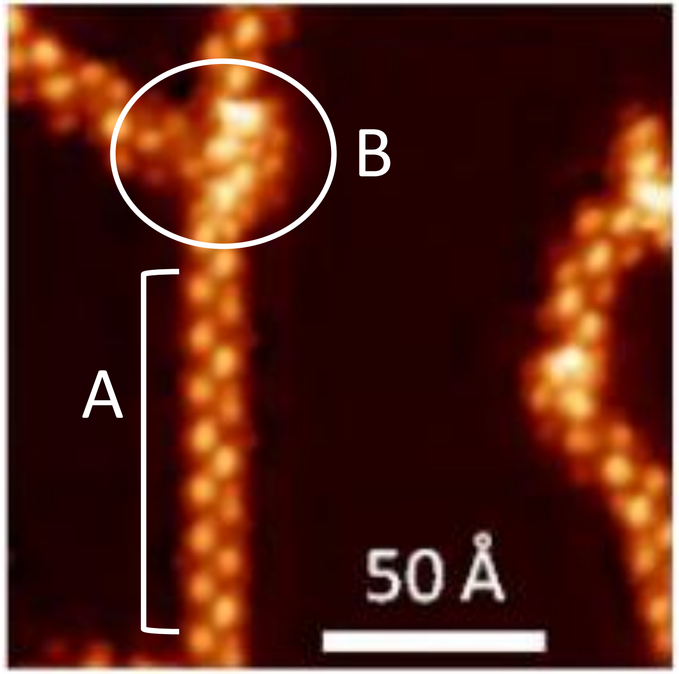
Island 1

+



Island 2

Experiment (30ºC)

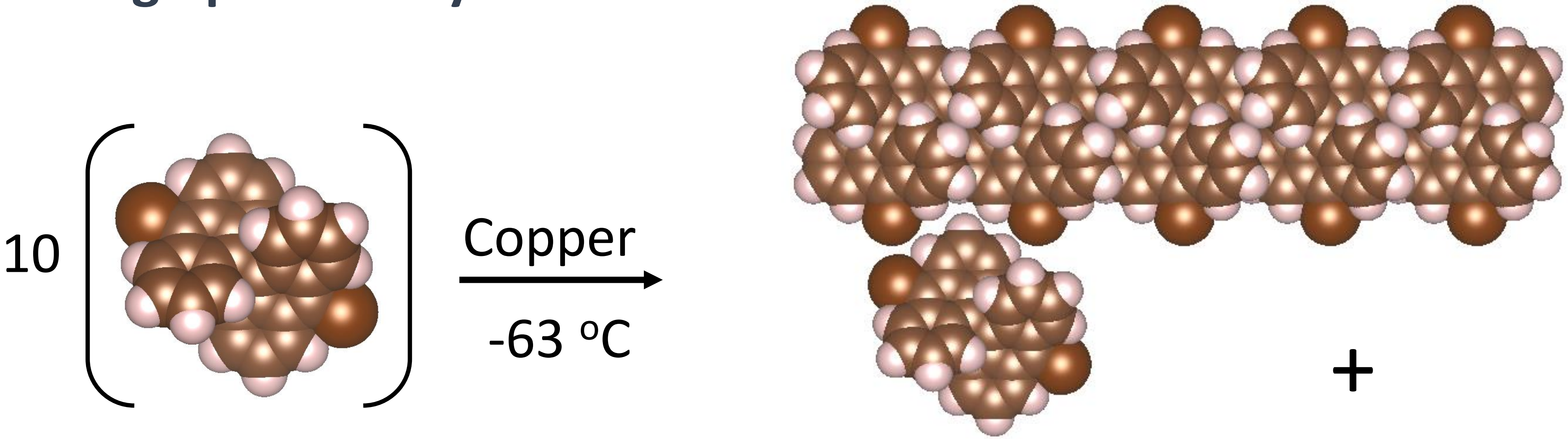


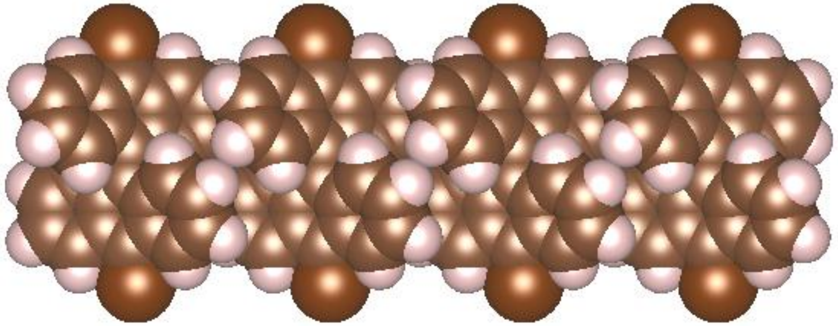
Good: Wire-shaped islands seen in experiment (A).

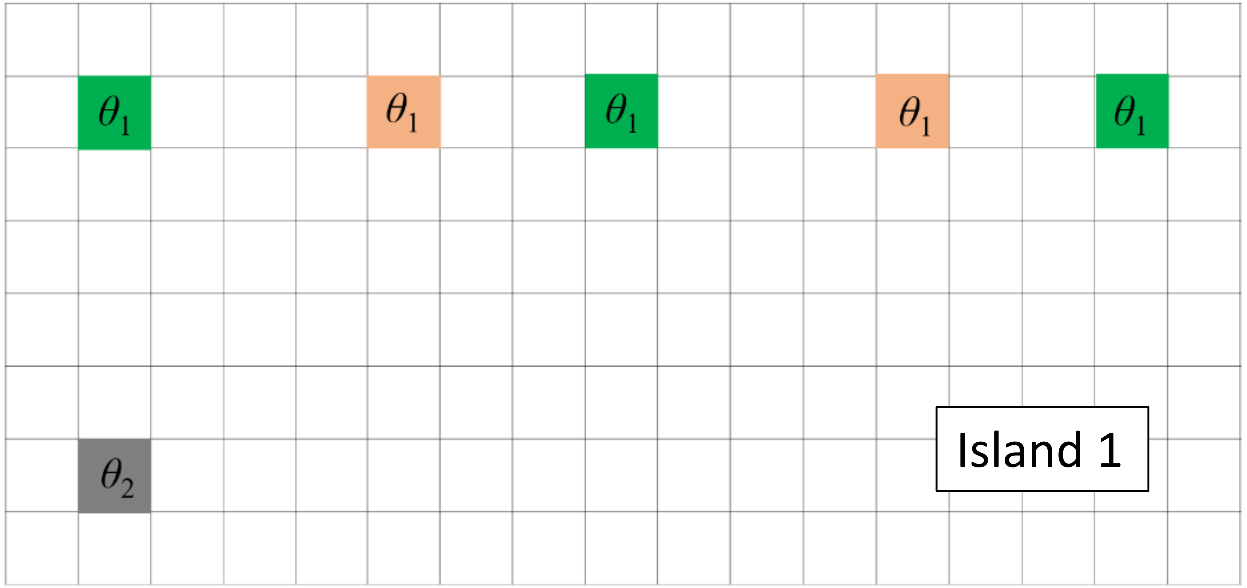
But: What about the part in (B)?

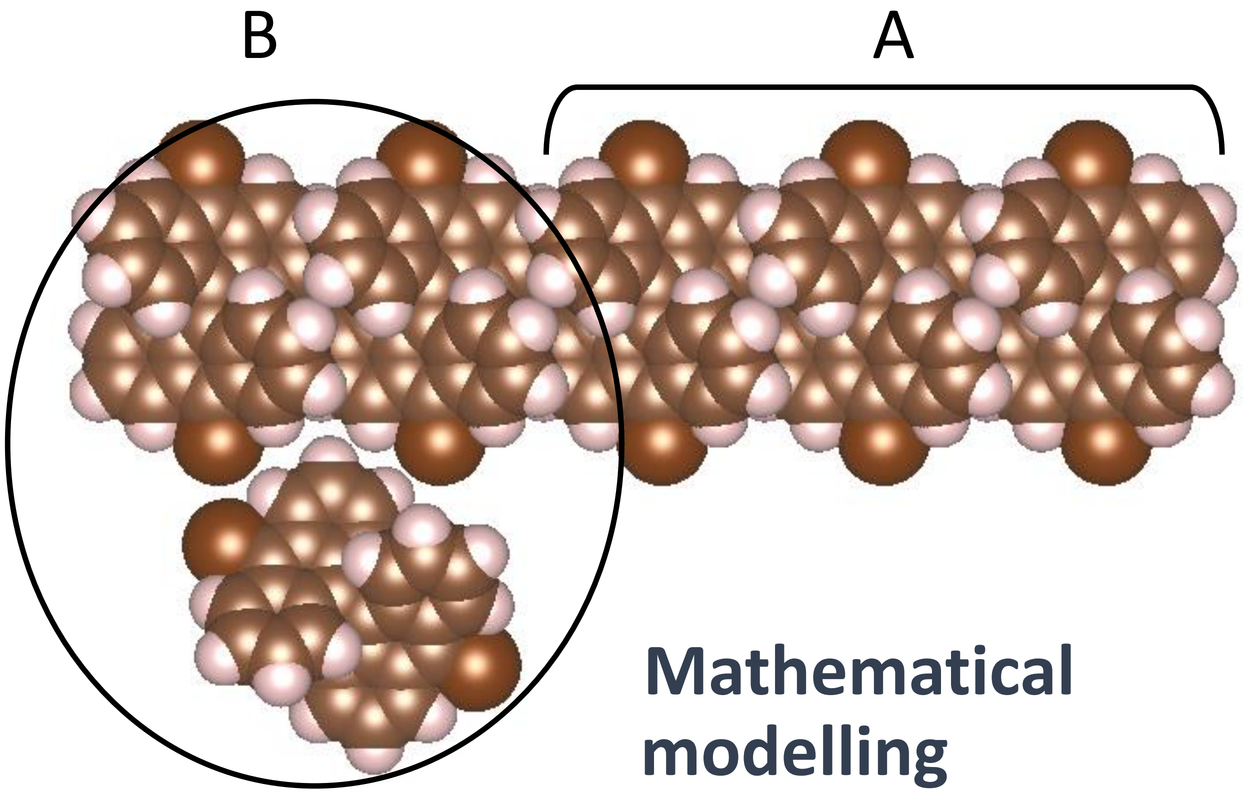
Let's consider a higher temperature…

High probability islands

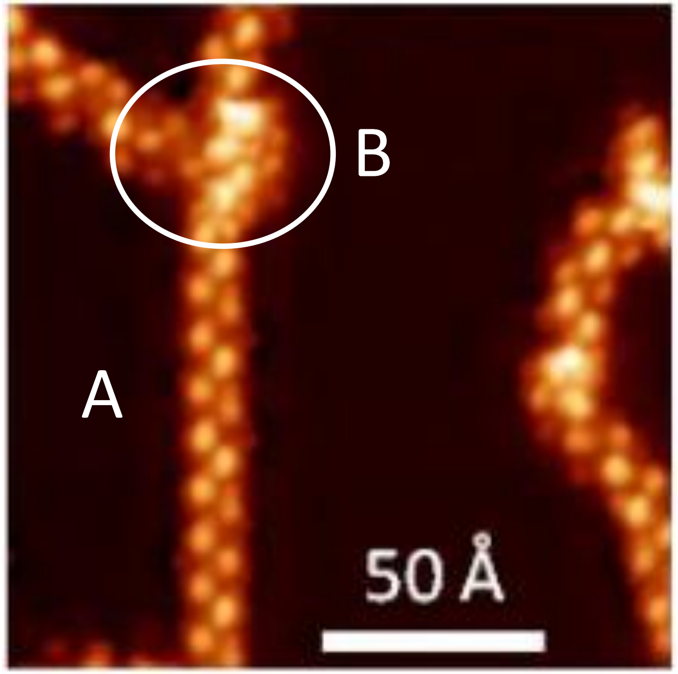








Mathematical modelling

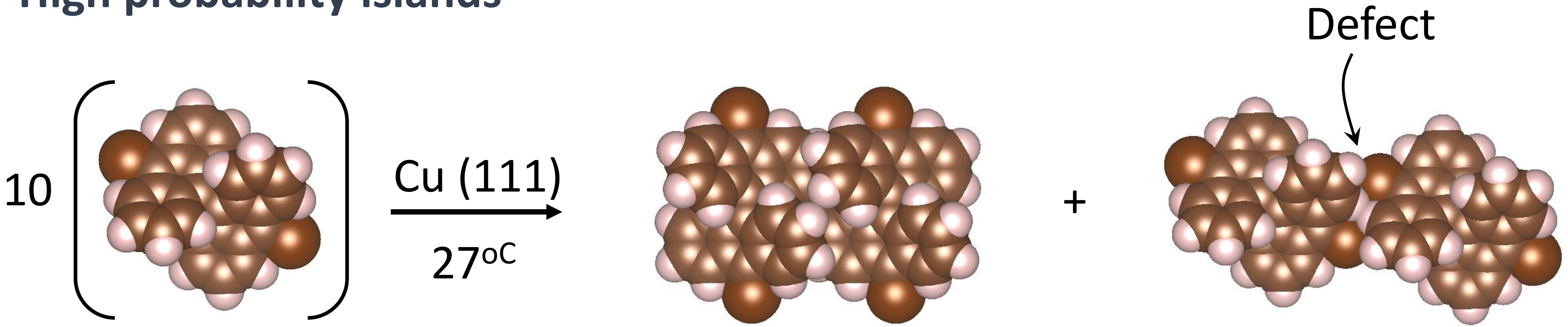


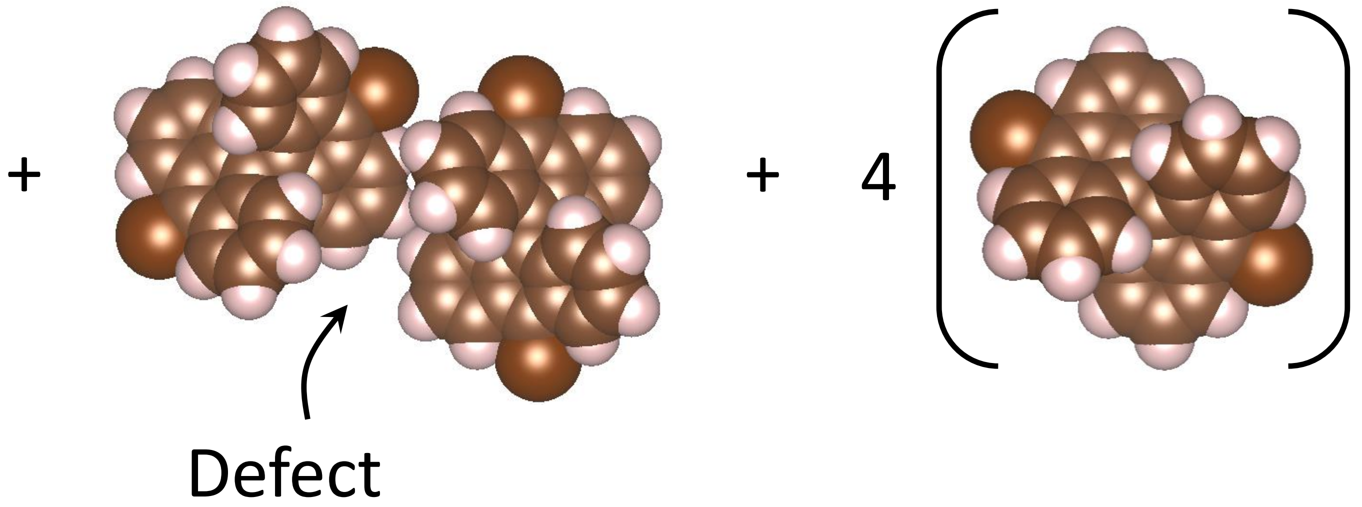
Experiment

At higher temperatures, mathematical modeling predicts similar feature to (B).

What about even higher temperatures?

High probability islands

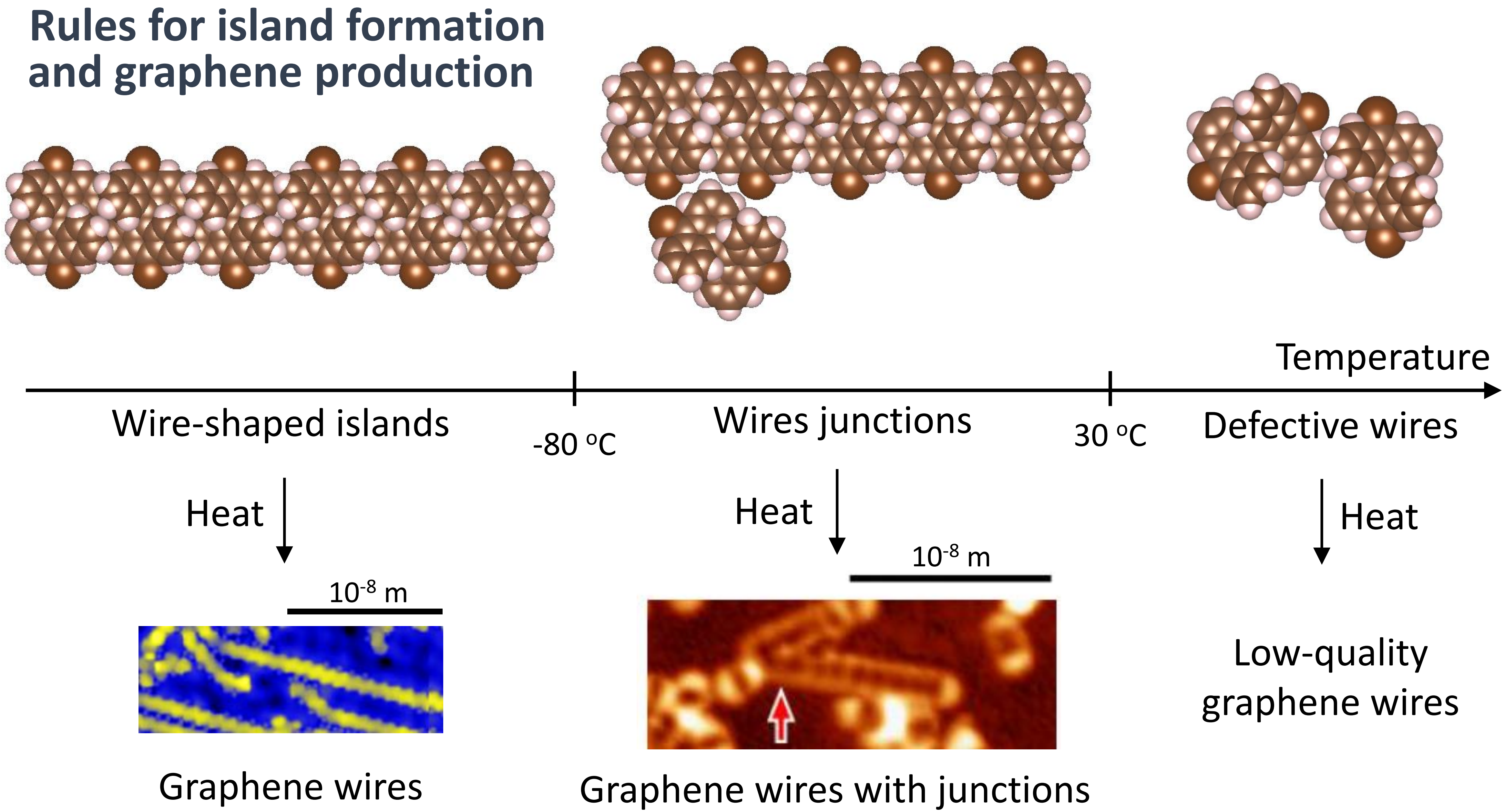




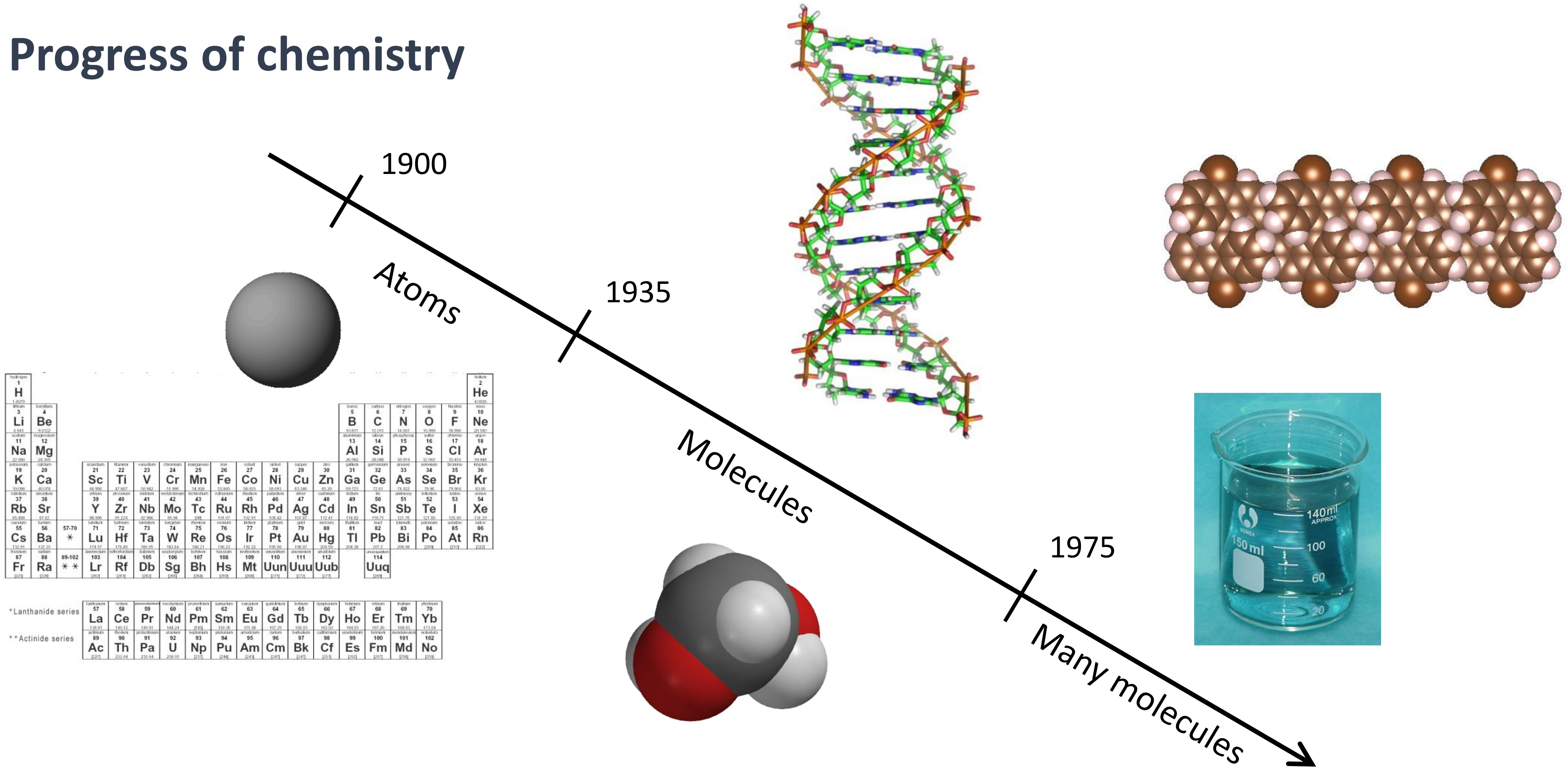
Island formation does not occur so much.

Islands are **short wires** with **defects**

Now, the rule starts to appear….


Rules for island formation
and graphene production
Temperature
Wire-shaped islands
-80 °C
Wires junctions
30 °C
Defective wires
Heat
Heat
Heat
10^-8 m
10^-8 m
Low-quality
graphene wires
Graphene wires
Graphene wires with junctions

Progress of chemistry



Rules concerning atoms and single molecules are **well understood**

Rules for interactions between molecules are **poorly understood**.

Mathematical modeling is necessary for progress in science.

Can you help? Study mathematics and science at high school and university.

Study them hard!

Study them critically and carefully!

Study them enthusiastically!

Acknowledgements

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