

# 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)

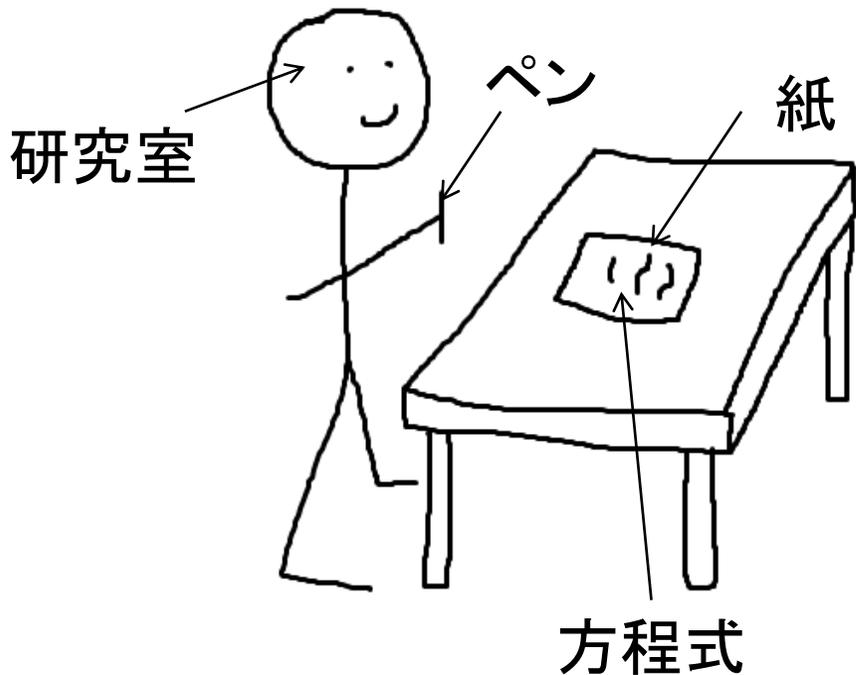
東北大学 原子分子材料科学高等研究機構

科学技術振興機構 さきがけ



東北大学



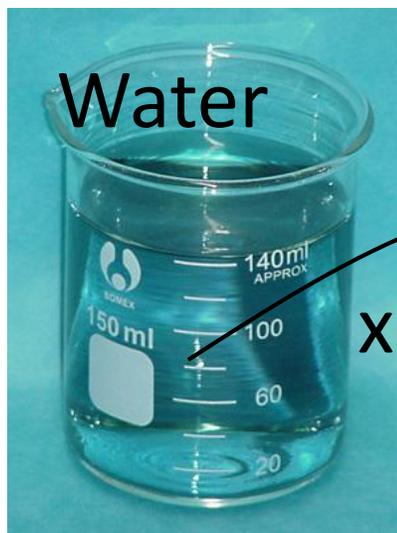


I am a **chemist** and an **applied mathematician**.

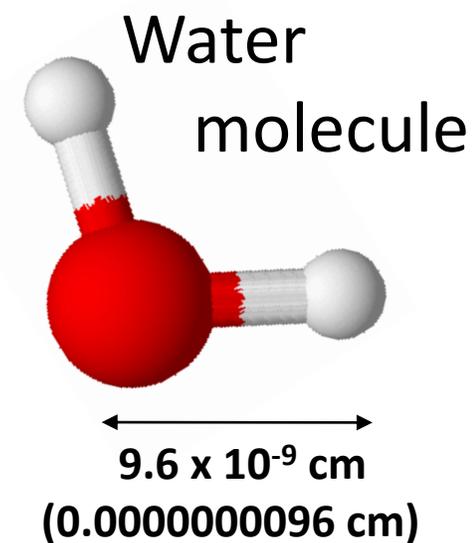
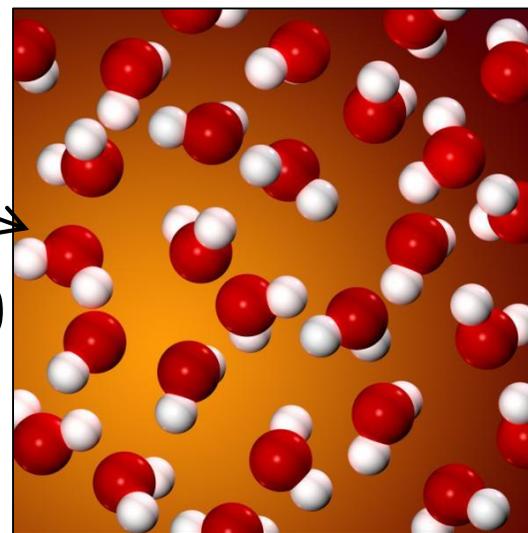
Chemistry = Science of creating new materials using molecules

Applied Mathematics = Science of abstracting natural phenomena

Molecules make up matter

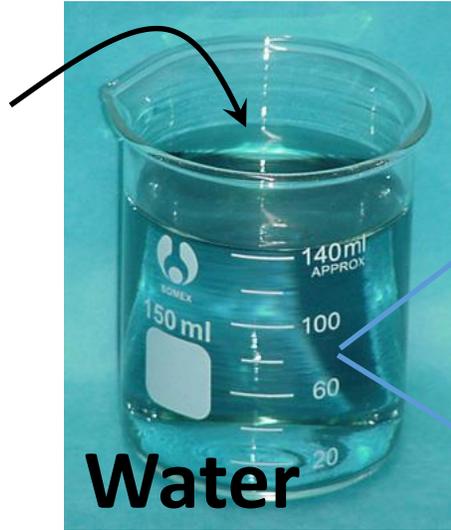
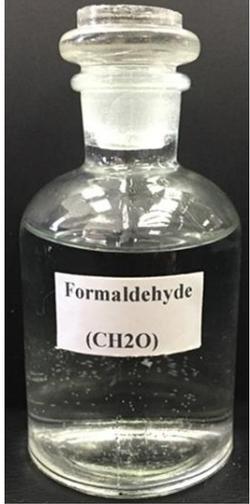


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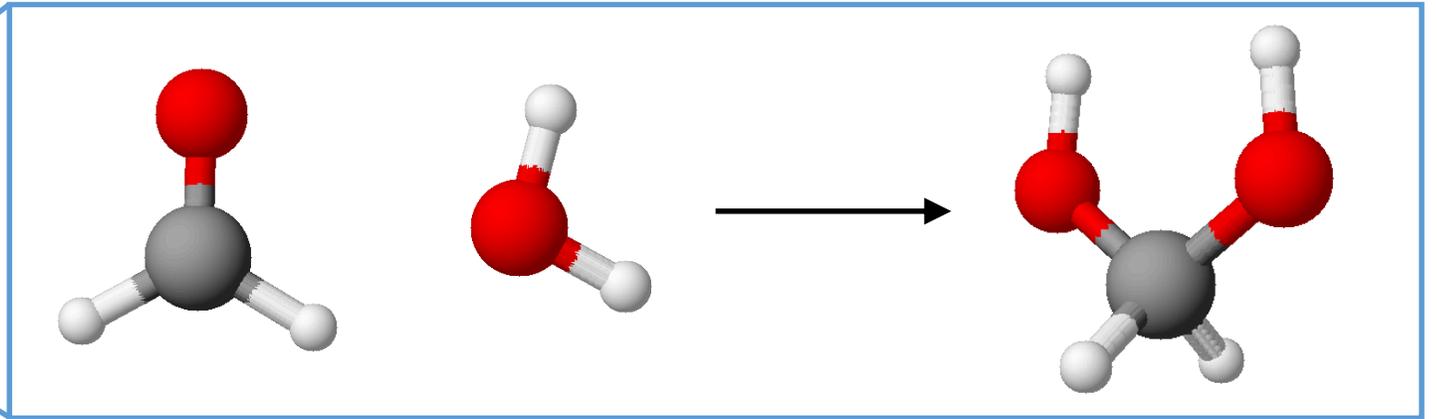


# How to make new materials using molecules?

1. Chemists mix molecules together.



2. Molecules **interact** with each other



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

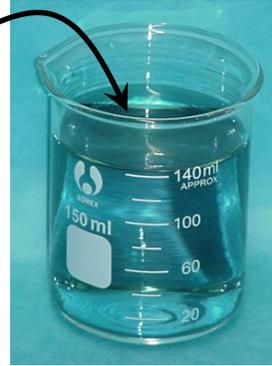
Chemists **can control** this step

Chemists **cannot control** this step!

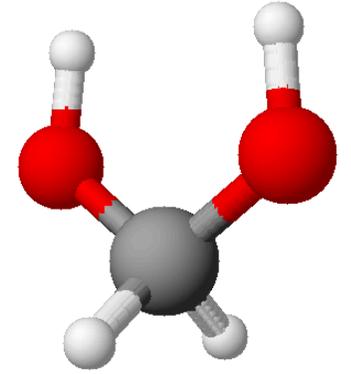
**Key point:** Before mixing the molecules together, chemists must **know the rules** for how the molecules will interact.

## What is a rule?

A 'rule' predicts what happens *without* doing an experiment.



Rule



## How to deduce new rules?

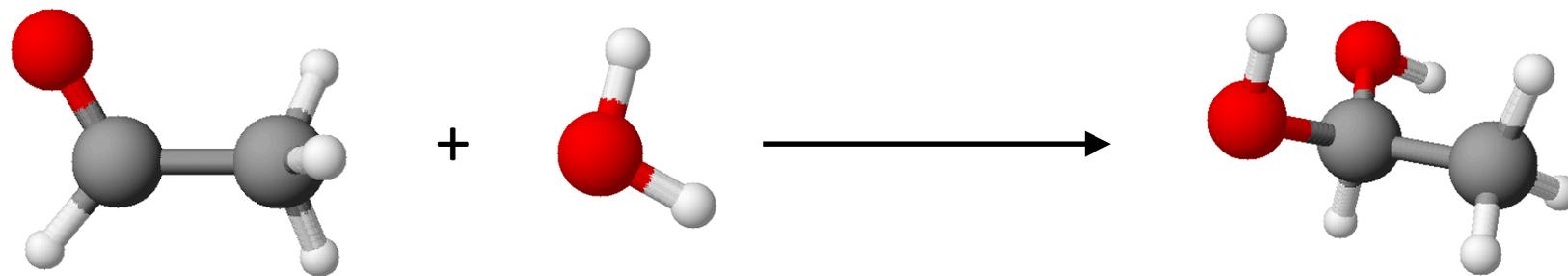
This is very difficult.

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

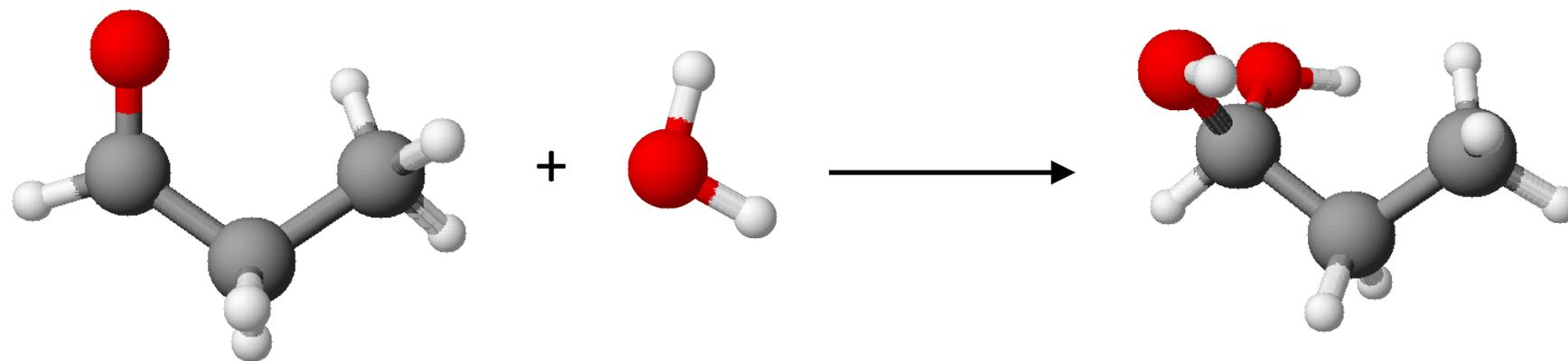


# Example: Let's deduce a rule!

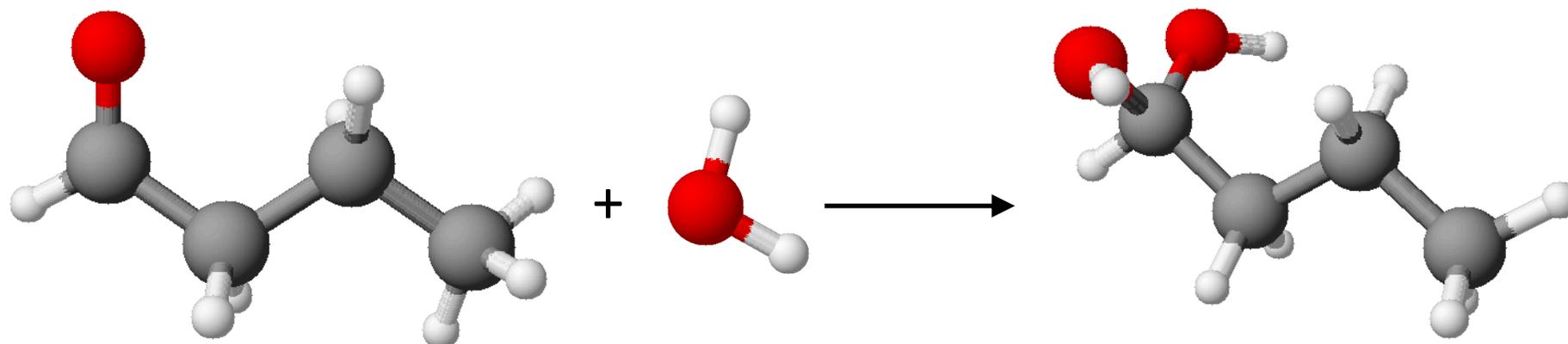
Experiment 1



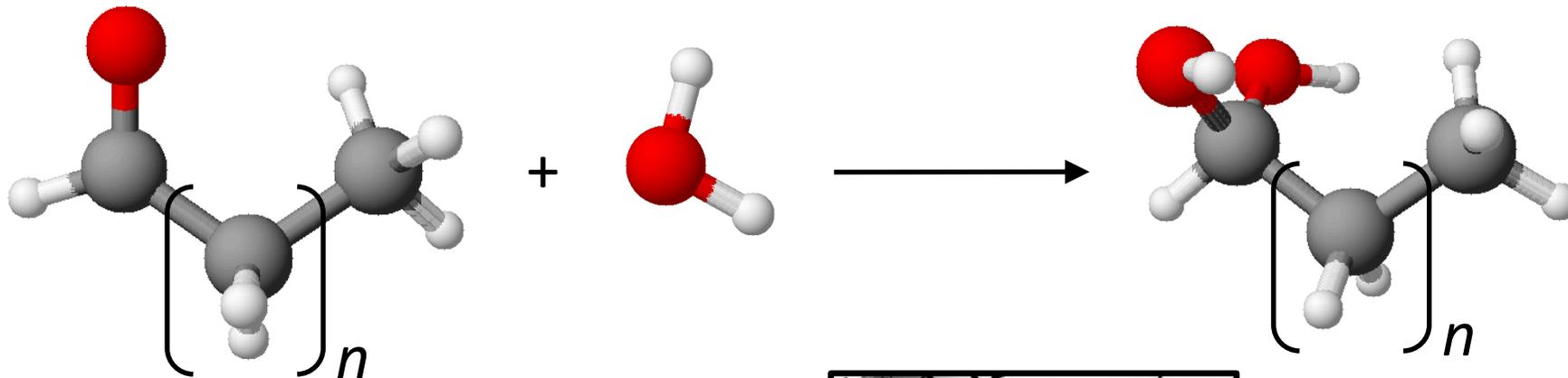
Experiment 2



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:

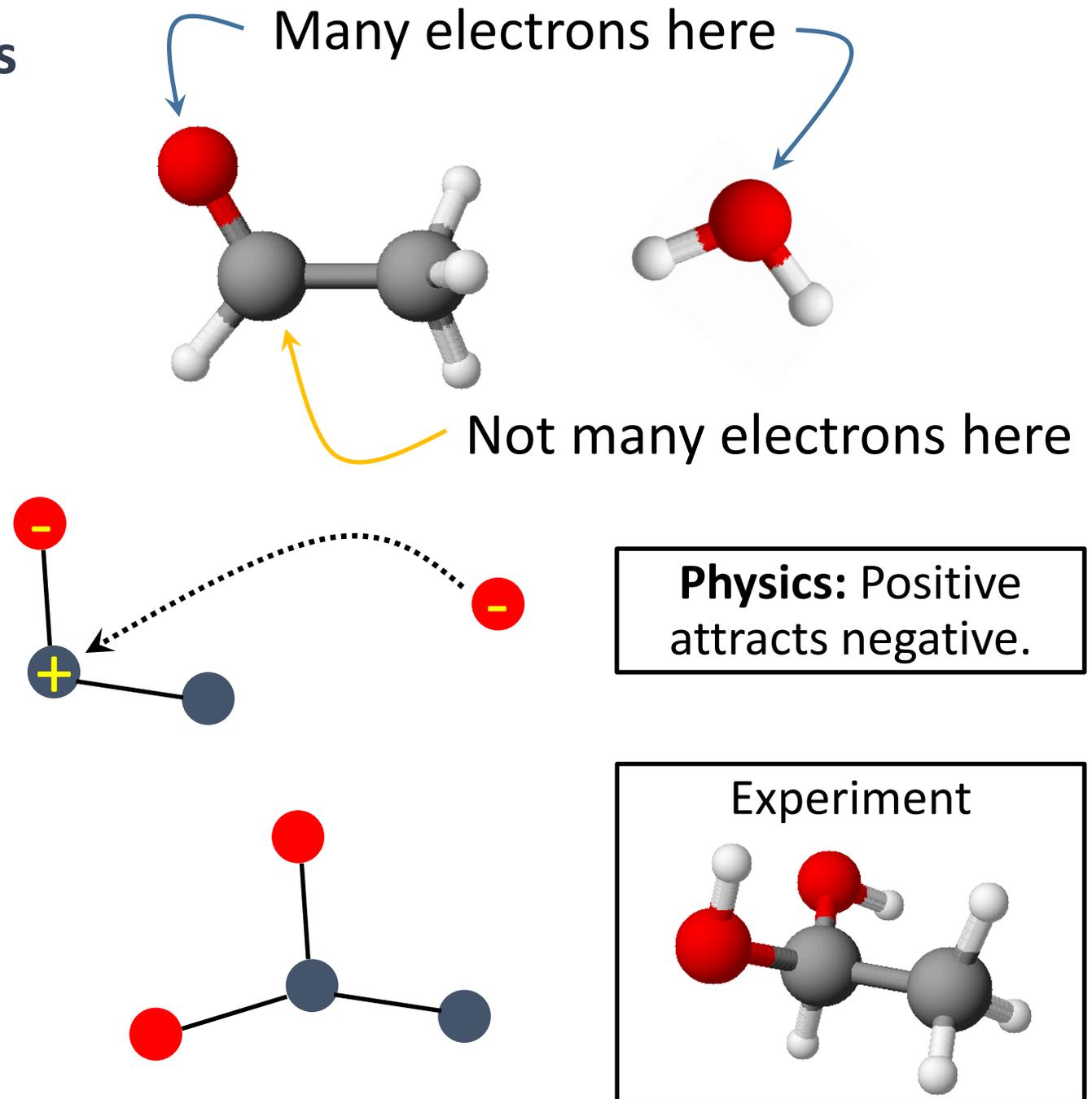
2. **Abstract** the real situation

3. Apply the **laws of physics**

→ Tells us the rule

4. Compare to **experiment**

**Similar** → Rule seems reasonable.



# Key Steps for Mathematical Modeling

1. Identify the key parts of the real situation

2. Abstract the real situation

3. Apply the laws of physics

4. Compare to experiment

Need a good knowledge of the situation!

Need to be good at mathematics!

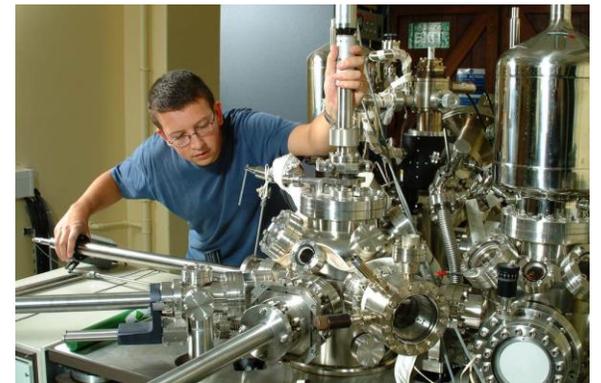
Need friends who can do experiments!

Periodic Table of the Elements

Legend:

- Alkali Metal
- Alkaline Earth
- Transition Metal
- Basic Metal
- Semimetal
- Nonmetal
- Halogen
- Noble Gas
- Lanthanide
- Actinide

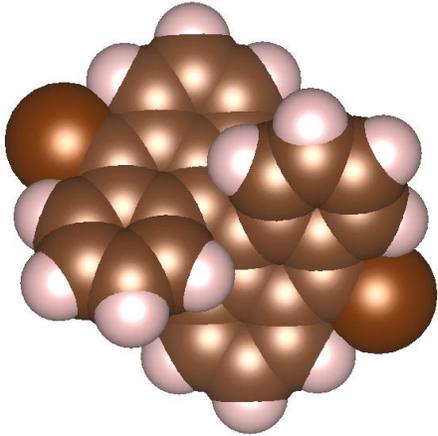
$$\frac{dX_t}{dt} = f(X_t) + b \frac{dW_t}{dt}$$



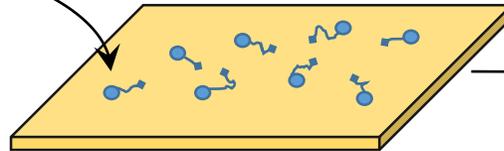
# Mathematical modelling for next-generation electrical materials

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

Di-bromo bi-anthryl (DBBA) molecule

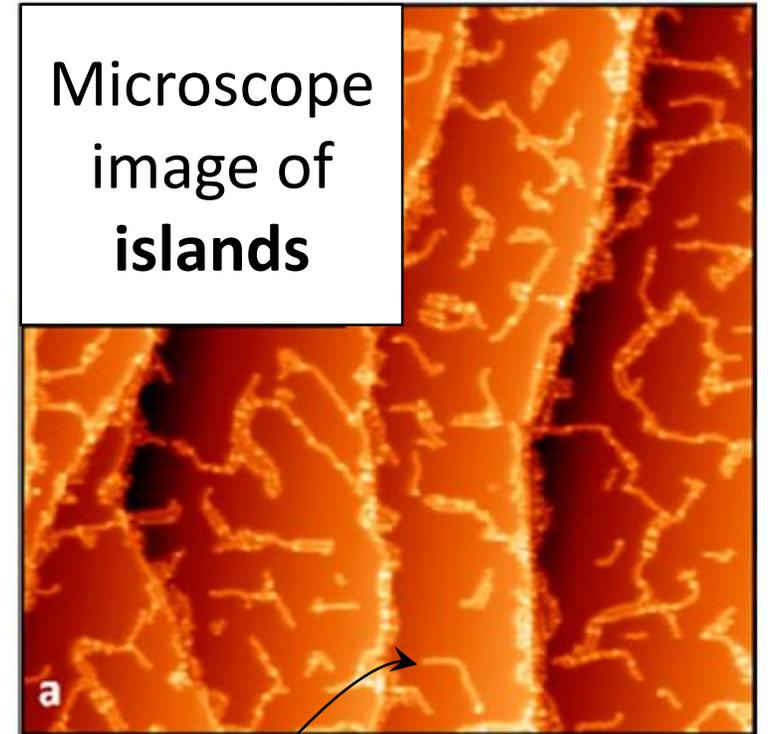


Place on copper surface

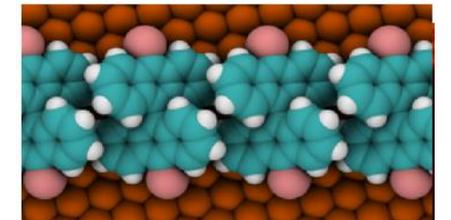


Molecules diffuse on surface

← 1.380 x 10<sup>-7</sup>m →



'Molecule island'

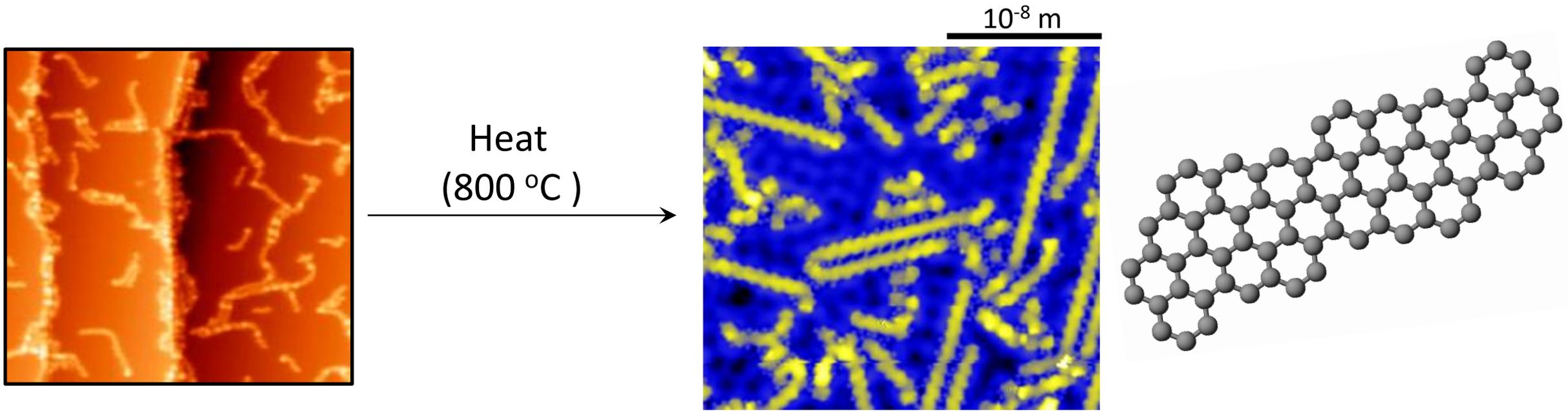


## What happened?

The molecules **assembled into islands**.

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

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



Islands turn into **graphene**

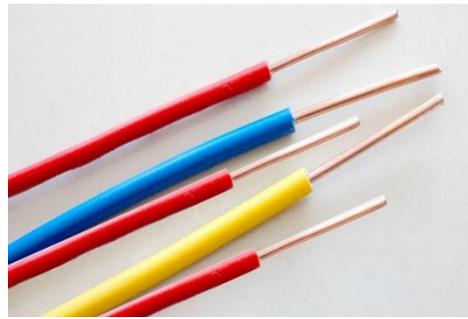
## What is special about graphene?

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

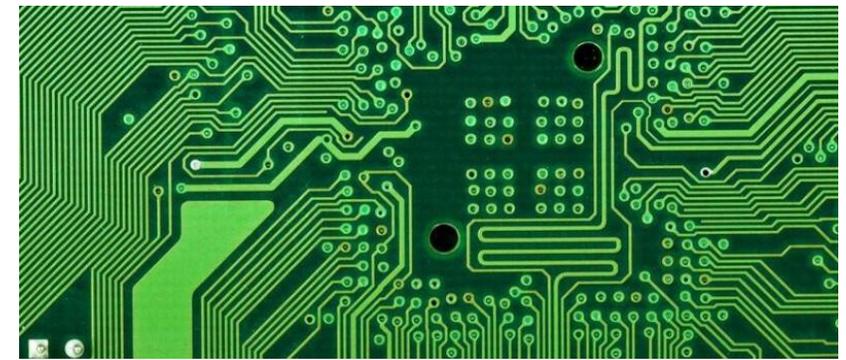
**Dream:** Create **real electronics** using graphene (e.g., extremely fast computers).

How might we make real electronics using graphene?

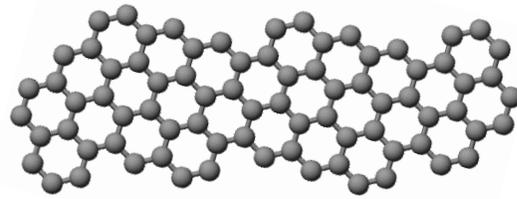
Wire:



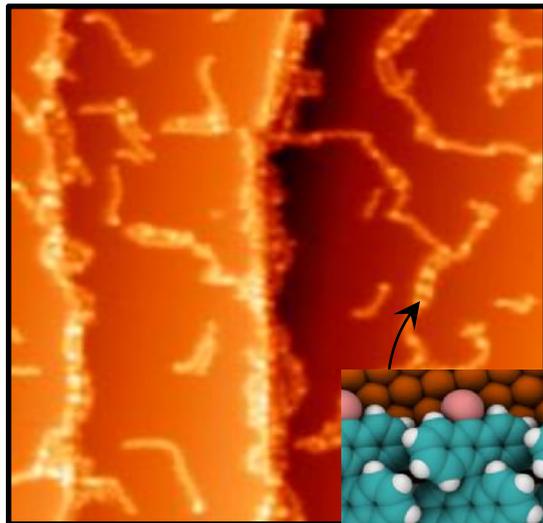
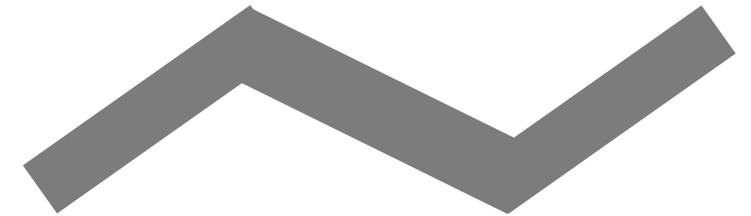
Electronic circuit:



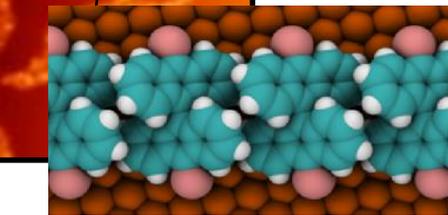
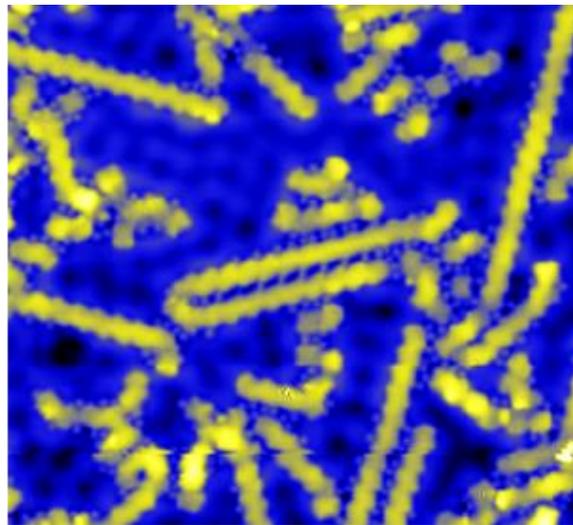
Wire-shaped graphene



Non-straight wires



Heat islands to 800 °C



Wire-shaped island

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

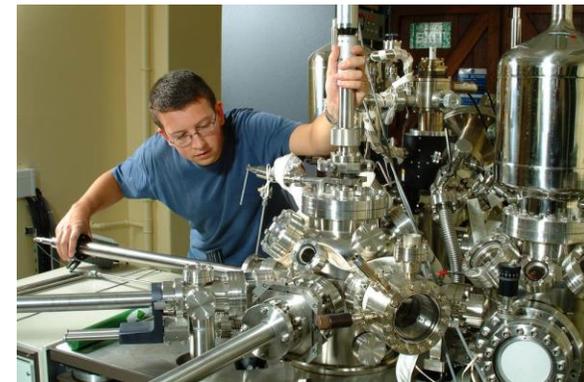
4. Compare to experiment

Periodic Table of the Elements

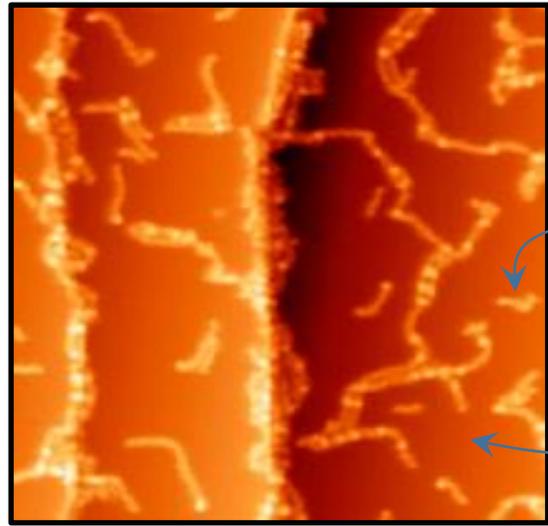
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- Alkali Metal
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$$\frac{dX_t}{dt} = f(X_t) + b \frac{dW_t}{dt}$$

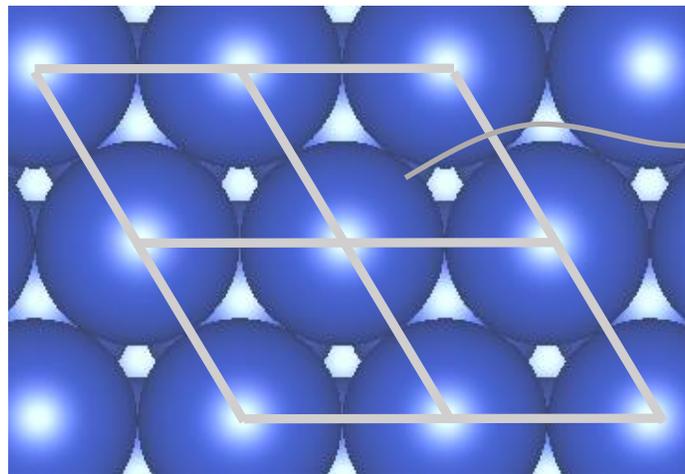
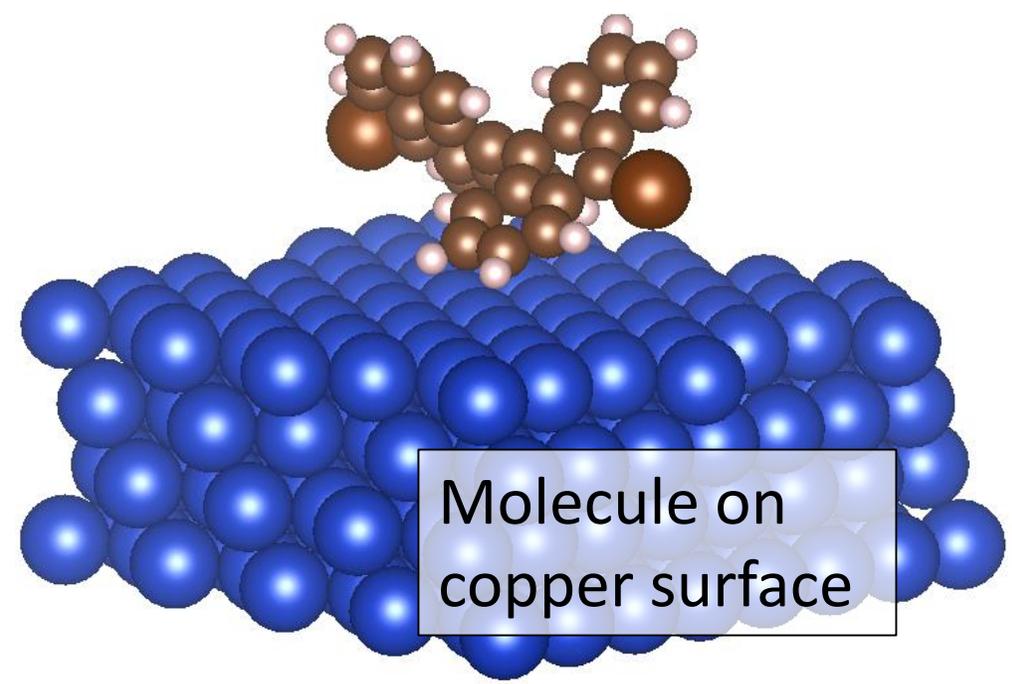


# 1. Key parts of the real situation

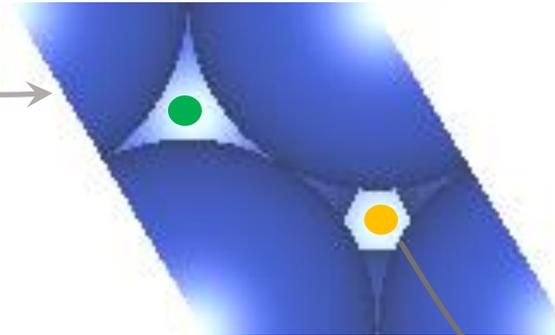


Island made of molecules

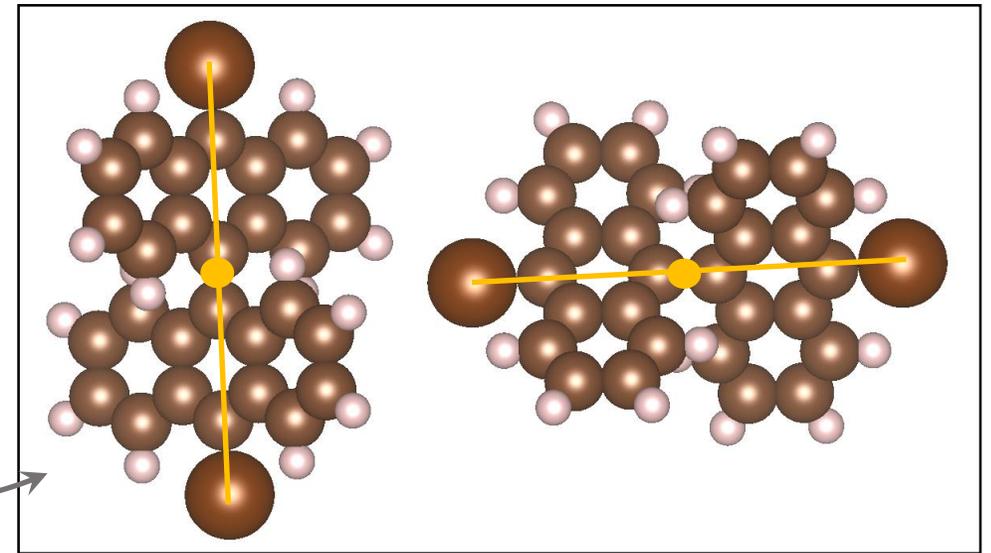
Copper surface



Unit cells of metal surface



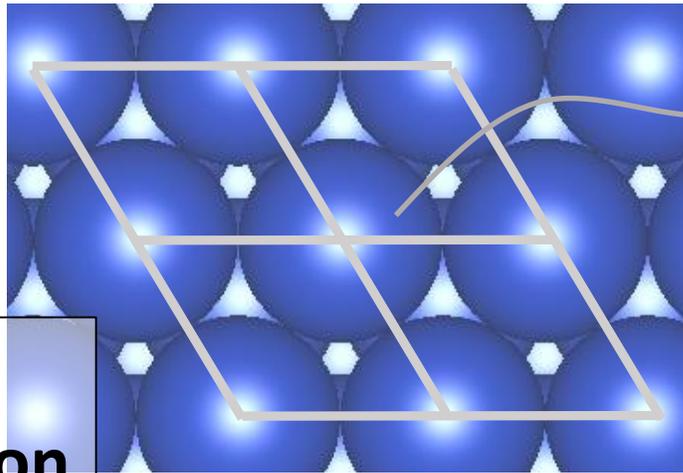
Adsorption sites



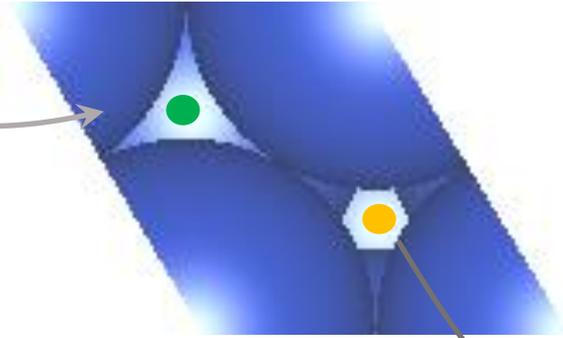
Molecule orientations

## 2. Abstract the real situation

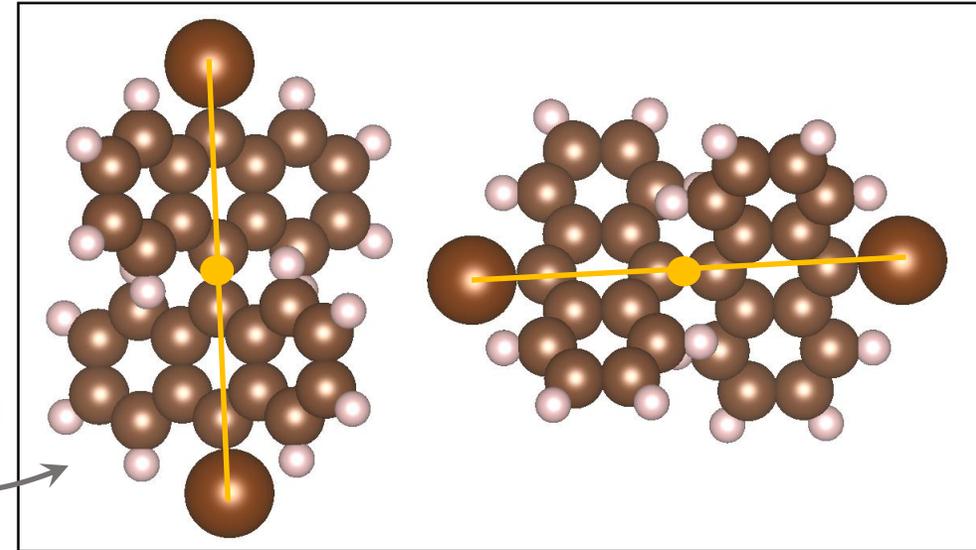
**Real situation**



Unit cells of metal surface

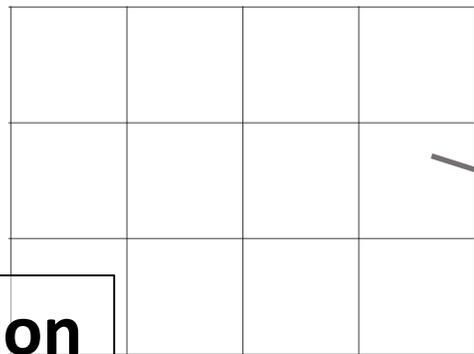


Adsorption sites



Molecule orientations

**Abstraction**

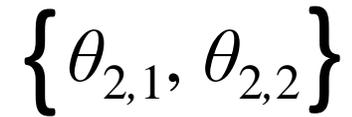


'Cells'  $C_1, C_2, \dots, C_M$



'Colours'

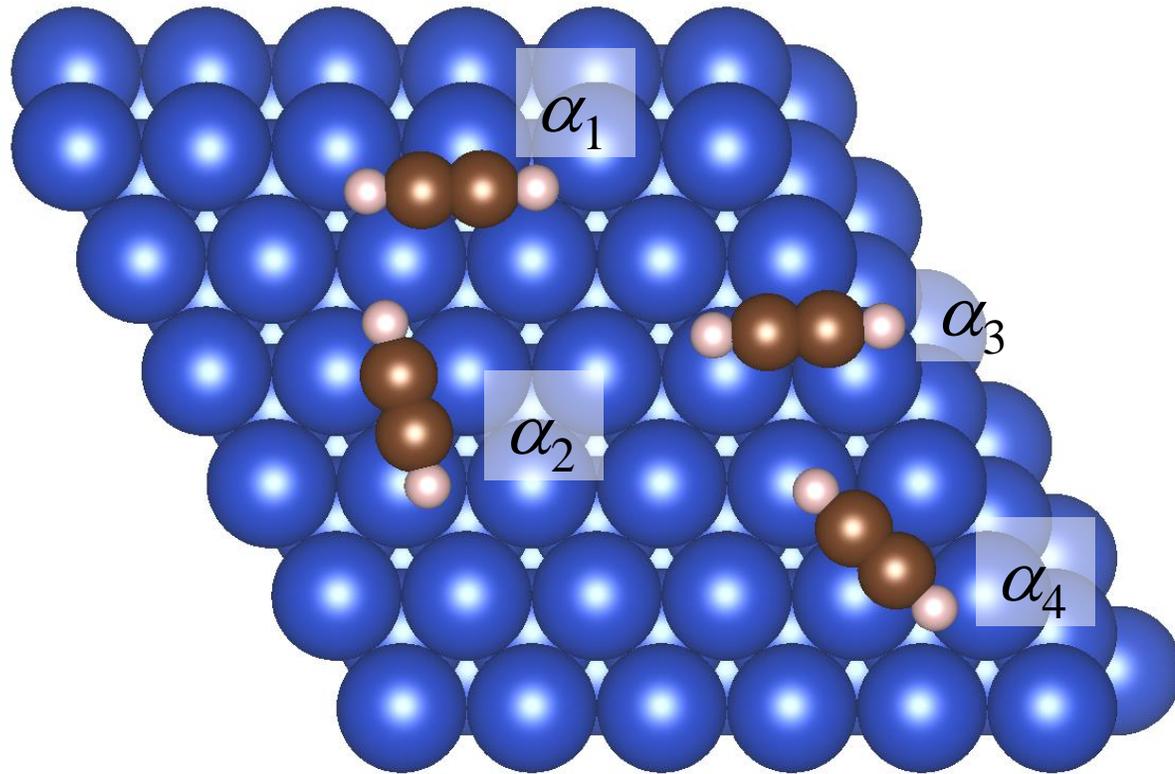
$\sigma_1, \sigma_2, \dots, \sigma_k$



'Shades'

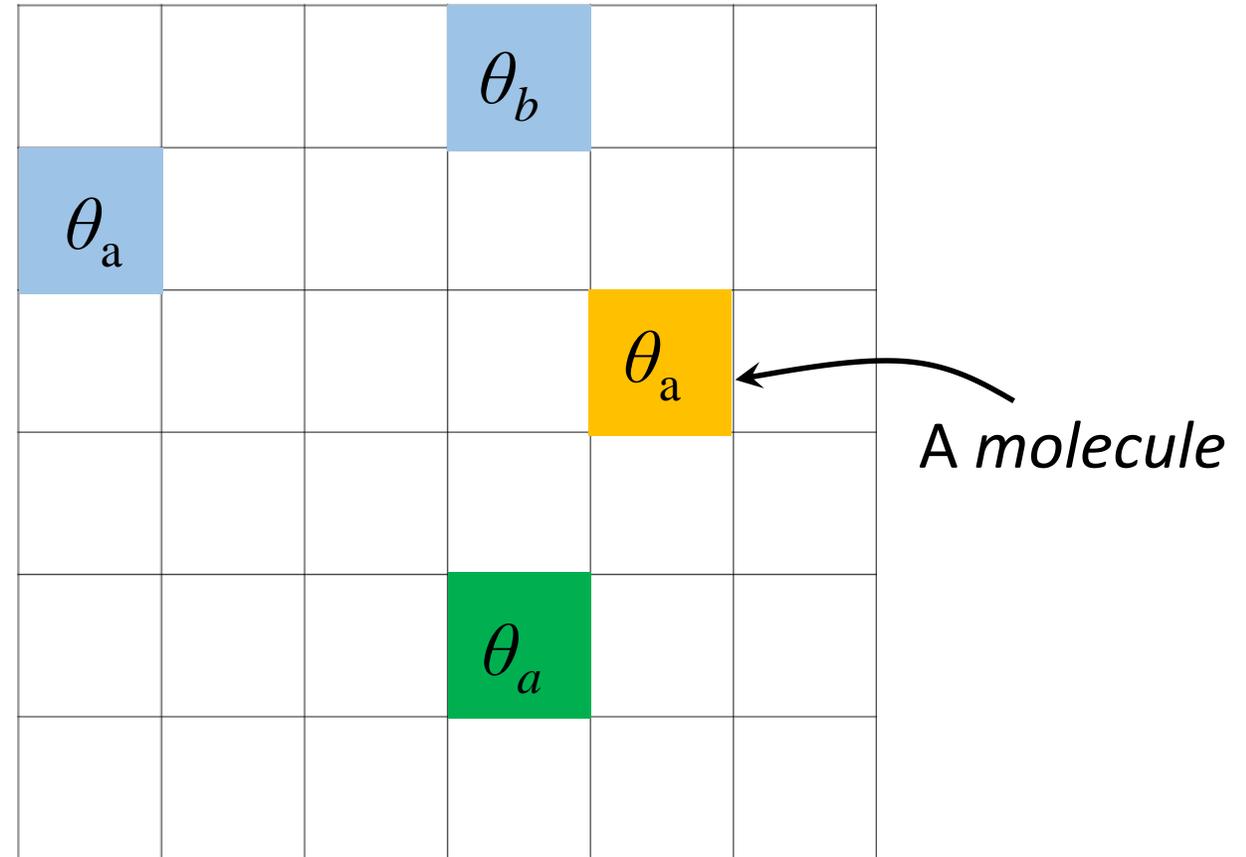
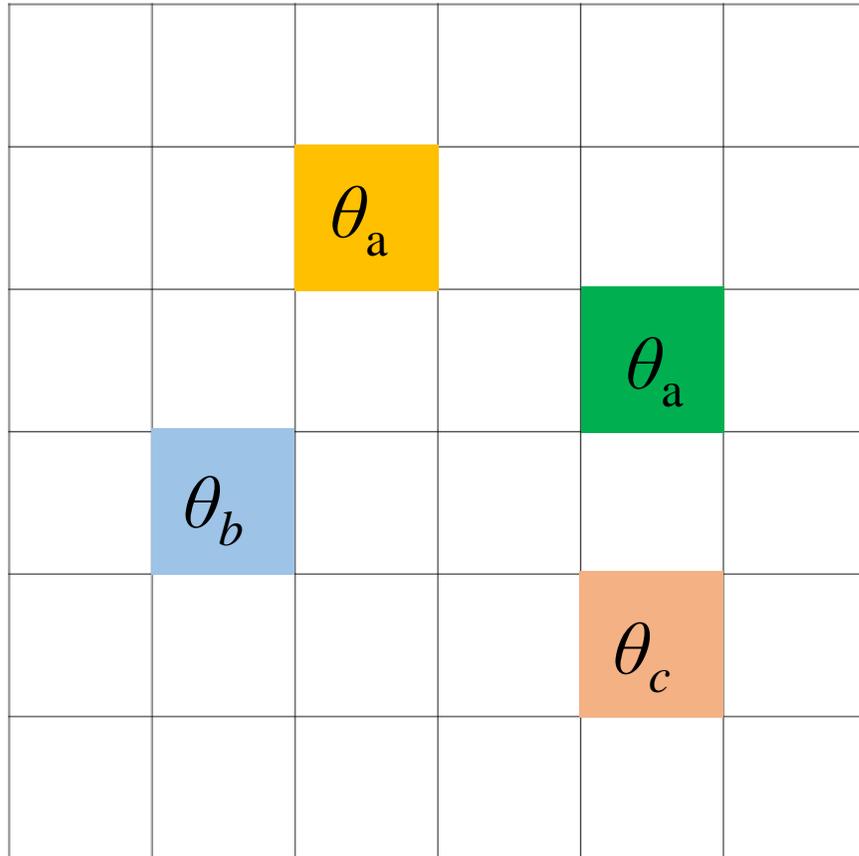
$\theta_{i,1}, \theta_{i,2}, \dots, \theta_{i,n(i)}$

# Reality – abstraction correspondence



		$\theta_a$	$\alpha_1$		
				$\theta_a$	$\alpha_3$
	$\theta_b$	$\alpha_2$			
				$\theta_c$	$\alpha_4$

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



Two configurations ( $N = 4$ , four colors  $\bullet \color{blue}\bullet \color{green}\bullet \color{orange}\bullet$ , three shades  $\theta_a, \theta_b, \theta_c$ )

# Mathematical modeling for island formation

- ✓ 1. Identify the key parts of the real situation.
- ✓ 2. Abstract the real situation

Periodic Table of the Elements

Atomic Number	Symbol	Name	Atomic Mass		
1	H	Hydrogen	1.008		
2	He	Helium	4.003		
3	Li	Lithium	6.941		
4	Be	Beryllium	9.012		
5	B	Boron	10.811		
6	C	Carbon	12.011		
7	N	Nitrogen	14.007		
8	O	Oxygen	15.999		
9	F	Fluorine	18.998		
10	Ne	Neon	20.180		
11	Na	Sodium	22.990		
12	Mg	Magnesium	24.305		
13	Al	Aluminum	26.982		
14	Si	Silicon	28.086		
15	P	Phosphorus	30.974		
16	S	Sulfur	32.065		
17	Cl	Chlorine	35.453		
18	Ar	Argon	39.948		
19	K	Potassium	39.098		
20	Ca	Calcium	40.078		
21	Sc	Scandium	44.956		
22	Ti	Titanium	47.887		
23	V	Vanadium	50.942		
24	Cr	Chromium	51.996		
25	Mn	Manganese	54.938		
26	Fe	Iron	55.845		
27	Co	Cobalt	58.933		
28	Ni	Nickel	58.693		
29	Cu	Copper	63.546		
30	Zn	Zinc	65.38		
31	Ga	Gallium	69.723		
32	Ge	Germanium	72.631		
33	As	Arsenic	74.922		
34	Se	Selenium	78.972		
35	Br	Bromine	79.904		
36	Kr	Krypton	84.358		
37	Rb	Rubidium	85.468		
38	Sr	Strontium	87.62		
39	Y	Yttrium	88.906		
40	Zr	Zirconium	91.224		
41	Nb	Niobium	92.906		
42	Mo	Molybdenum	95.95		
43	Tc	Technetium	98.907		
44	Ru	Ruthenium	101.07		
45	Rh	Rhodium	102.906		
46	Pd	Palladium	106.42		
47	Ag	Silver	107.868		
48	Cd	Cadmium	112.411		
49	In	Indium	114.818		
50	Sn	Tin	118.710		
51	Sb	Antimony	121.760		
52	Te	Tellurium	127.6		
53	I	Iodine	126.905		
54	Xe	Xenon	131.294		
55	Cs	Cesium	132.905		
56	Ba	Barium	137.328		
57-71	Lanthanide Series				
72	Hf	Hafnium	178.49		
73	Ta	Tantalum	180.948		
74	W	Tungsten	183.84		
75	Re	Rhenium	186.207		
76	Os	Osmium	190.23		
77	Ir	Iridium	192.222		
78	Pt	Platinum	195.085		
79	Au	Gold	196.967		
80	Hg	Mercury	200.592		
81	Tl	Thallium	204.383		
82	Pb	Lead	207.2		
83	Bi	Bismuth	208.980		
84	Po	Polonium	209		
85	At	Astatine	209		
86	Rn	Radon	222		
87	Fr	Francium	223		
88	Ra	Radium	226		
89-103	Actinide Series				
104	Rf	Rutherfordium	[261]		
105	Db	Dubnium	[262]		
106	Sg	Seaborgium	[266]		
107	Bh	Berkelium	[267]		
108	Hs	Hassium	[268]		
109	Mt	Moscovium	[268]		
110	Ds	Darmstadtium	[271]		
111	Rg	Roentgenium	[272]		
112	Cn	Copernicium	[285]		
113	Uut	Ununtrium	unknown		
114	Fu	Flerovium	unknown		
115	Uup	Ununpentium	unknown		
116	Lv	Livermorium	unknown		
117	Uus	Ununseptium	unknown		
118	Uuo	Ununoctium	unknown		

3. Apply the laws of physics

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

4. Compare to experiment



Let  $c$  be a configuration.

*Boltzmann distribution law* from physics

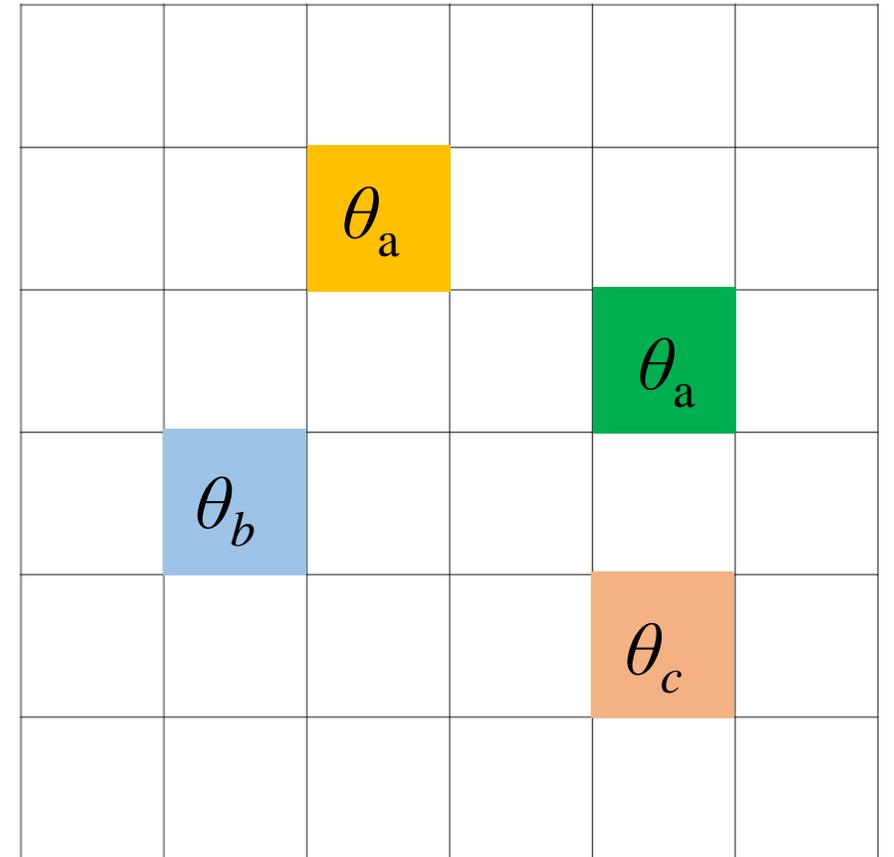
→ probability of configuration  $c$

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

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

$k_B$  = Boltzmann constant ( $1.38 \times 10^{-23}$  J K<sup>-1</sup>)

$T$  = Temperature

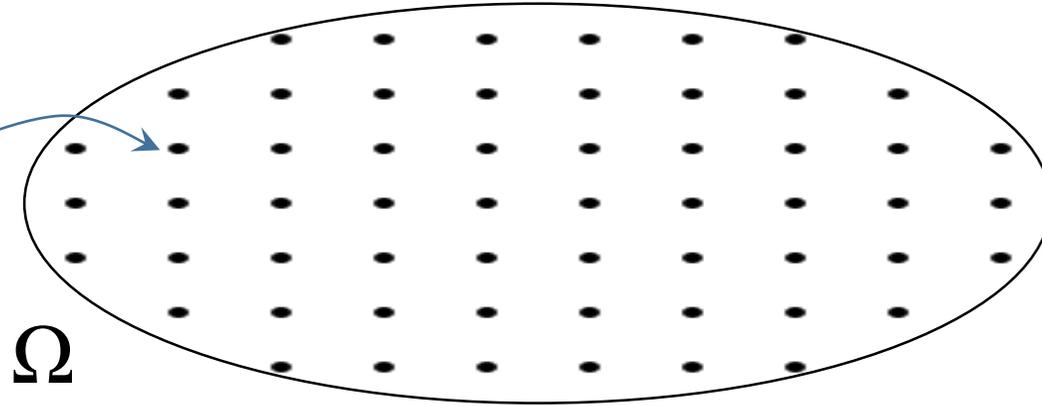
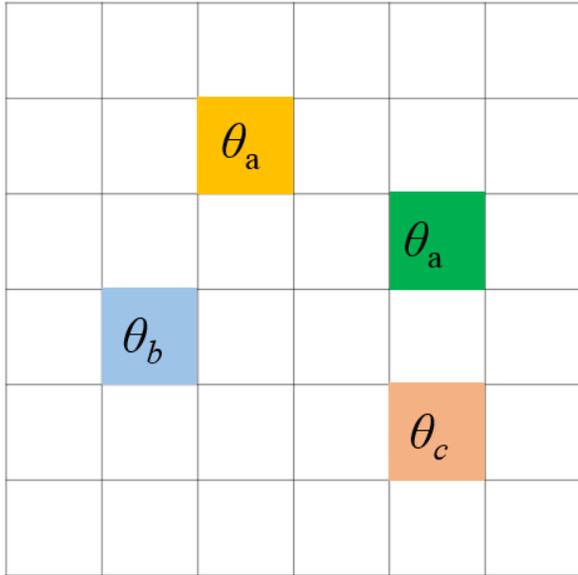


one configuration ( $c$ )

**Mathematical challenge**

Find configurations that have high probability.

## Search for High Probability Configurations



$\Omega =$  configuration space

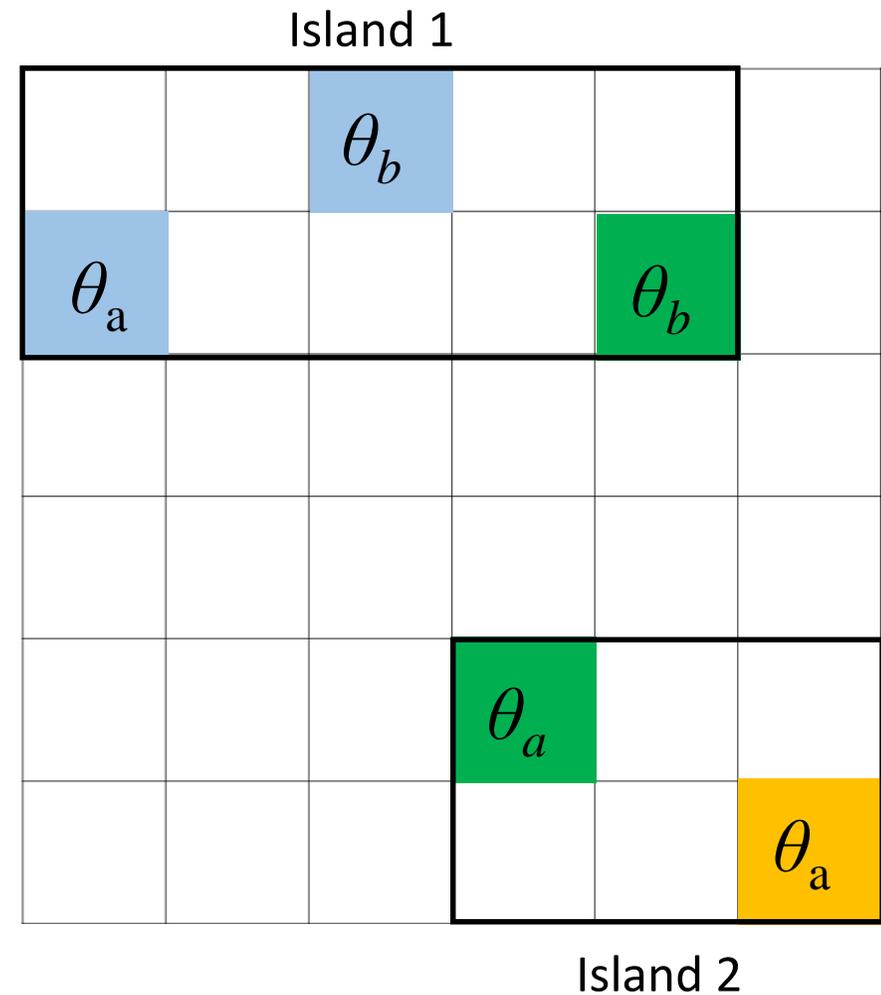
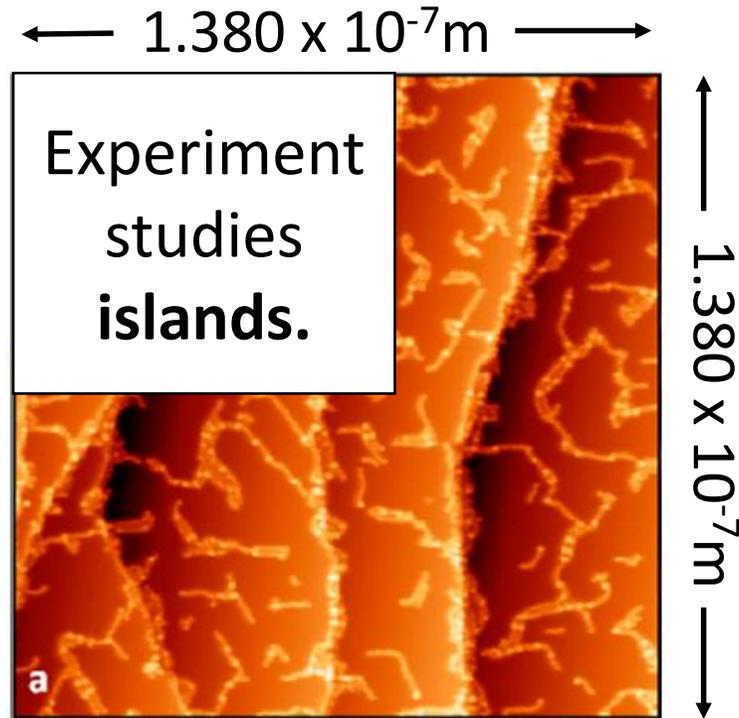
### Configuration space is extremely big!

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.

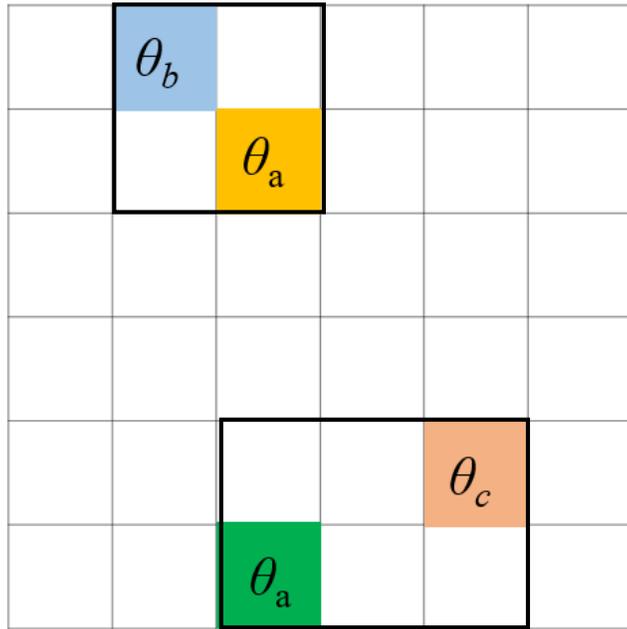
Then  $10^{23} \times 10^{-6}$  s  $\approx 10^{10}$  years to check probability for every configuration!

With mathematical thinking, a faster approach is possible...

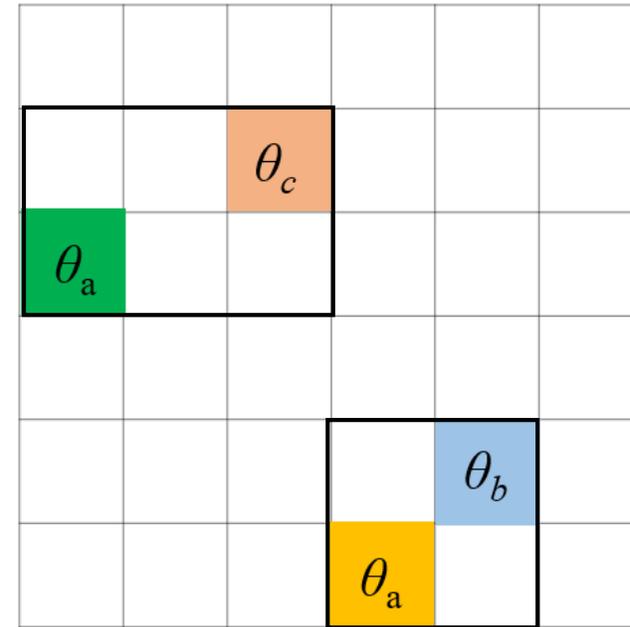
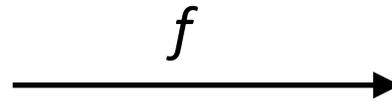


Mathematical definition of **islands**?

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**.

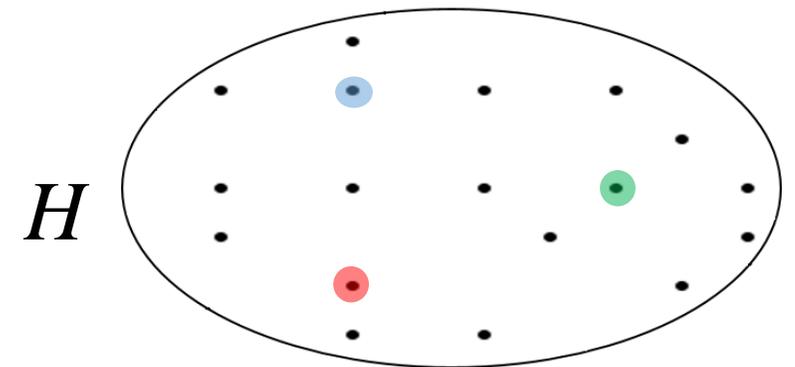
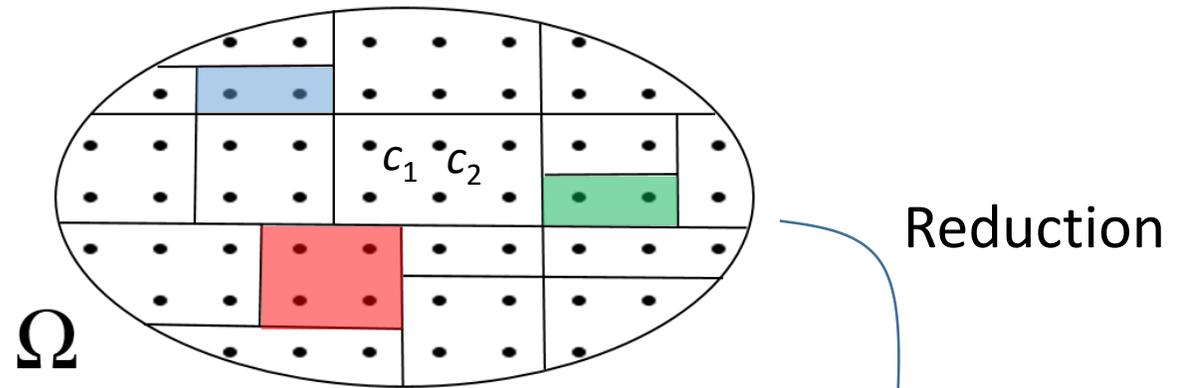
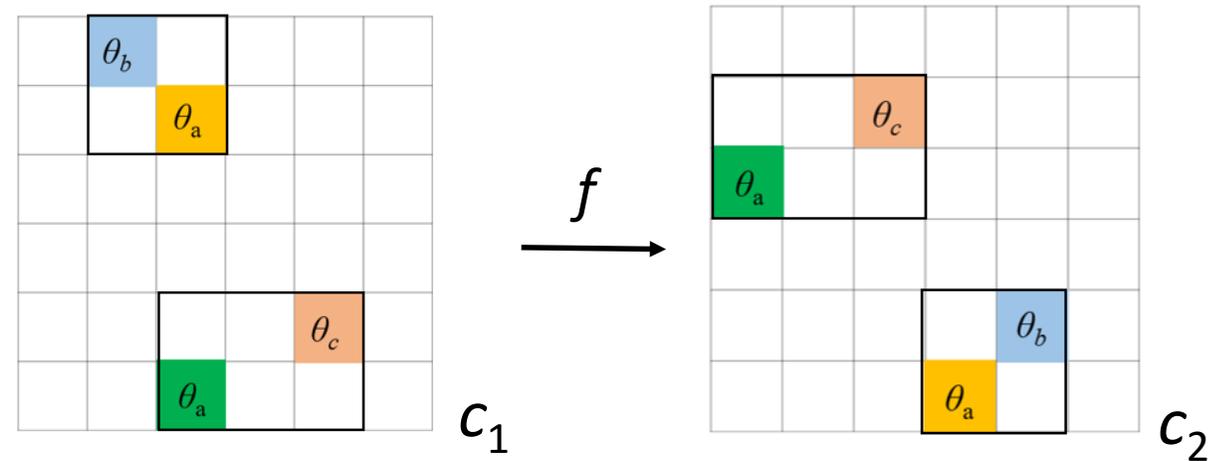
The isomorphism divides the configuration space into **equivalence classes**

Reduced space  $H$   
= collection of equivalence classes

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

(compare:  $\Omega$  has around  $10^{23}$  elements!)

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



# Mathematical modeling for island formation

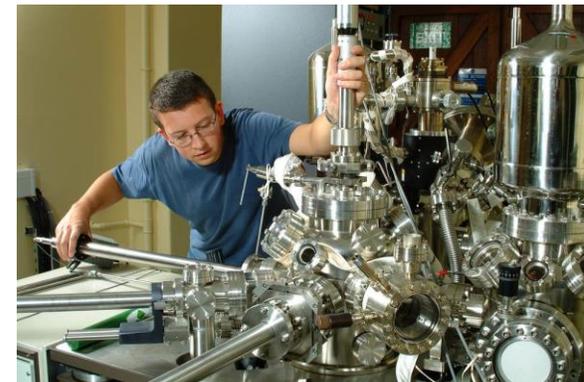
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Periodic Table of the Elements

Legend:

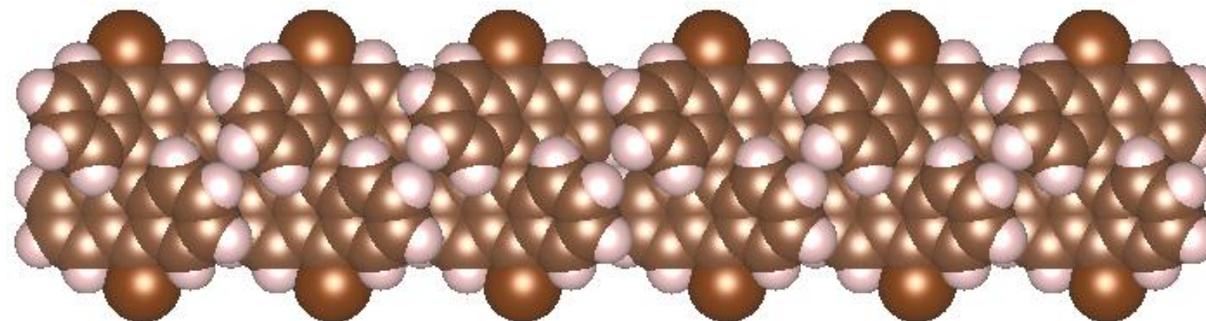
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- Nonmetal
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- Actinide

4. Compare to experiment



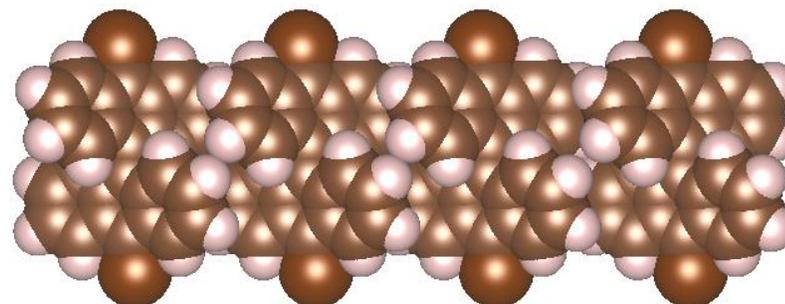


Mathematical  
modelling (-123°C)



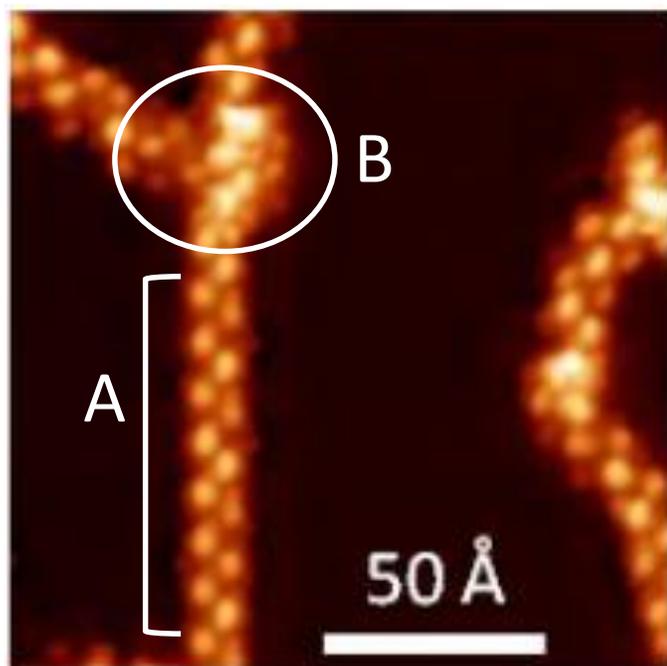
Island 1

+



Island 2

Experiment (30°C)

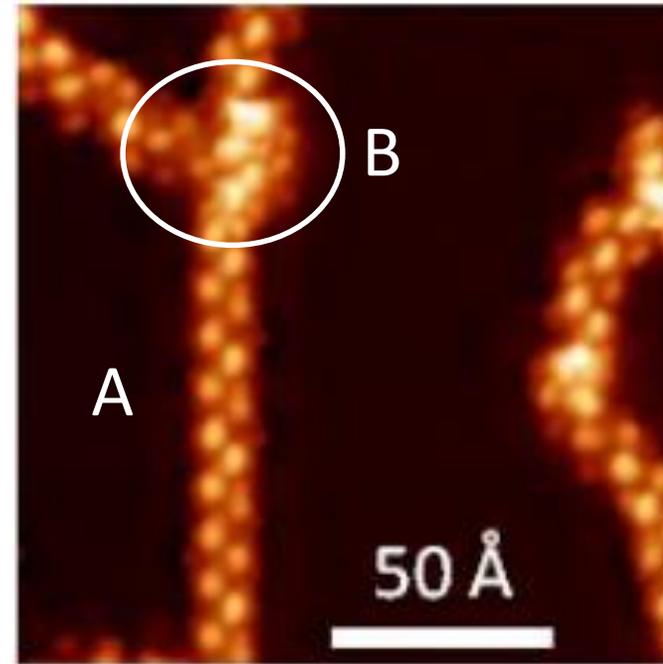
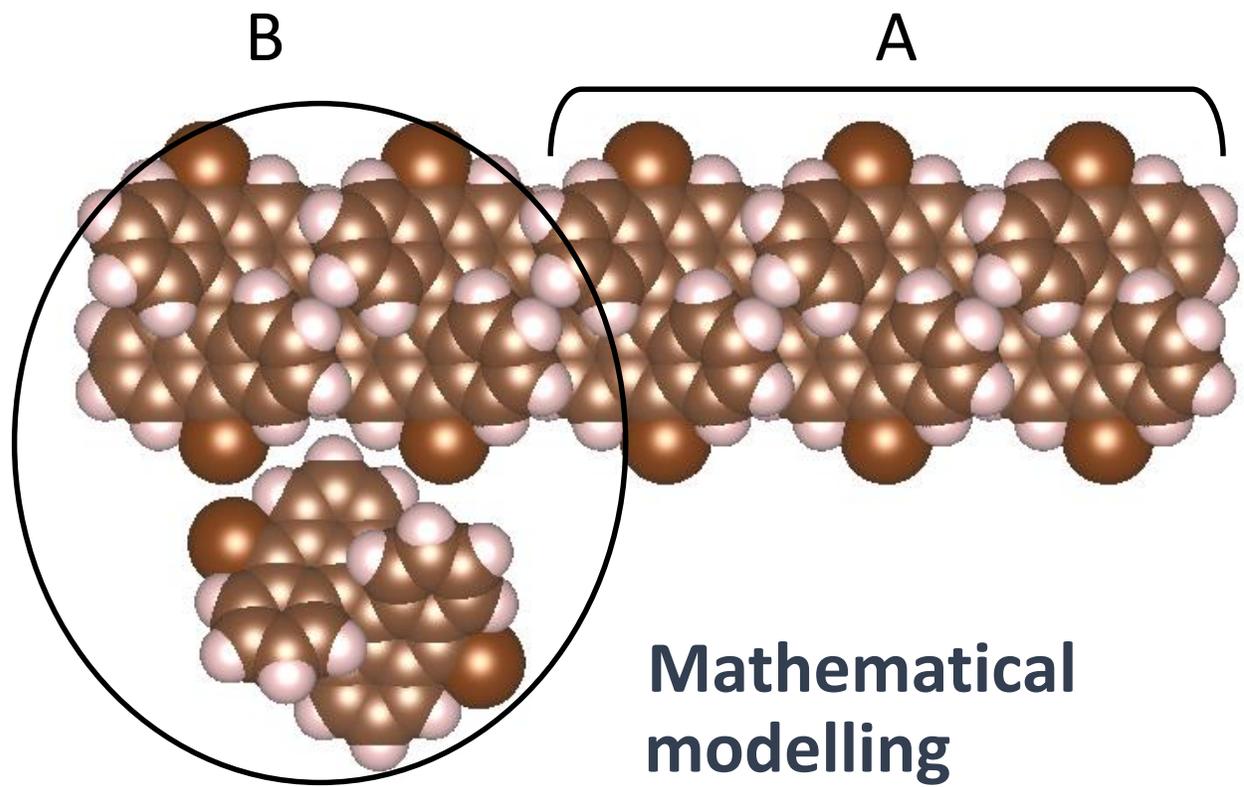


**Good:** Wire-shaped islands seen in experiment (A).

**But:** What about the part in (B)?

Let's consider a higher temperature...



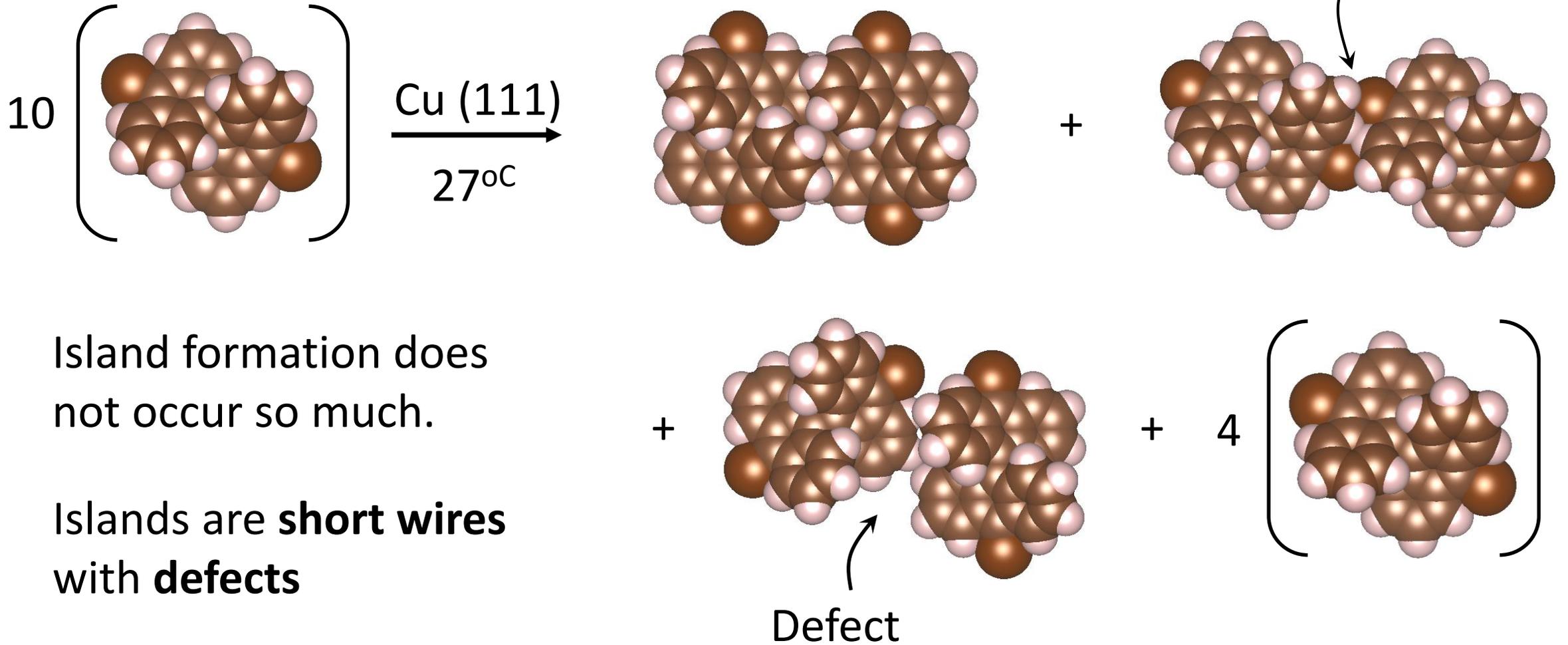


**Experiment**

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

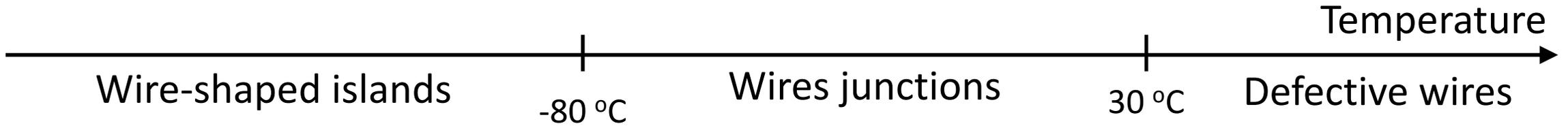
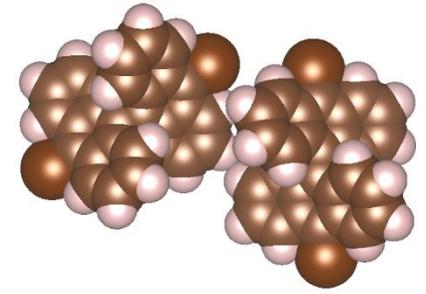
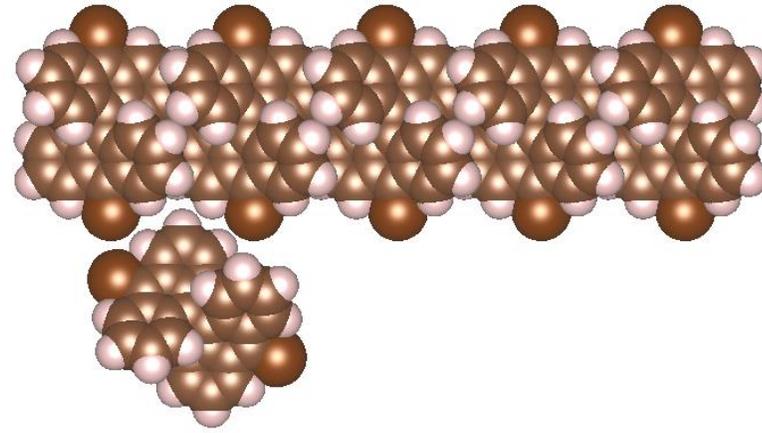
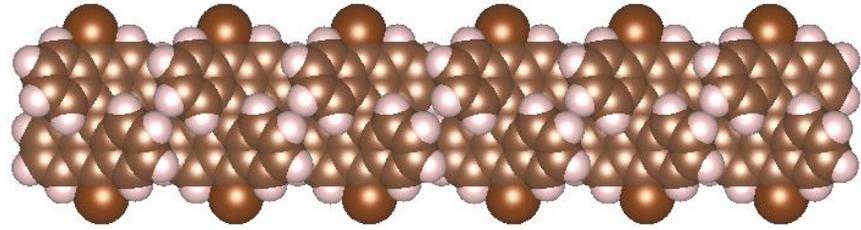
What about even higher temperatures?

# High probability islands



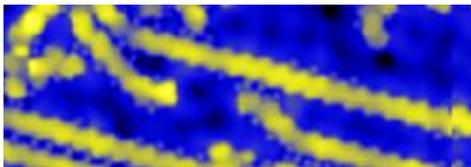
**Now, the rule starts to appear....**

# Rules for island formation and graphene production



Heat ↓

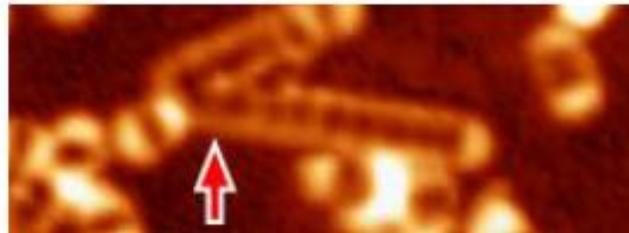
$10^{-8}$  m



Graphene wires

Heat ↓

$10^{-8}$  m



Graphene wires with junctions

Heat ↓

Low-quality  
graphene wires

# Progress of chemistry

1900

Atoms



Hydrogen 1 H 1.00794	Helium 2 He 4.002602
Lithium 3 Li 6.941	Beryllium 4 Be 9.012182
Sodium 11 Na 22.98976928	Magnesium 12 Mg 24.304
Potassium 19 K 39.0983	Calcium 20 Ca 40.078
Rubidium 37 Rb 85.4678	Sr 38 Sr 87.62
Cesium 55 Cs 132.90545196	Ba 56 Ba 137.327
Francium 87 Fr [223]	Ra 88 Ra [226]
Lanthanum 57 La 138.90547	Cerium 58 Ce 140.12
Actinium 89 Ac [227]	Thorium 90 Th 232.0377
	Protactinium 91 Pa 231.036888
	Uranium 92 U 238.02891
	Niobium 41 Nb 92.90638
	Molybdenum 42 Mo 95.94
	Technetium 43 Tc [98]
	Ruthenium 44 Ru 101.07
	Rhodium 45 Rh 102.90550
	Palladium 46 Pd 106.42
	Silver 47 Ag 107.8682
	Cadmium 48 Cd 112.414
	Indium 49 In 114.818
	Tin 50 Sn 118.710
	Antimony 51 Sb 121.757
	Tellurium 52 Te 127.6
	Iodine 53 I 126.90547
	Xenon 54 Xe 131.29
	Krypton 36 Kr 83.80
	Bromine 35 Br 79.904
	Selenium 34 Se 78.96
	Arsenic 33 As 74.9216
	Germanium 32 Ge 72.630
	Gallium 31 Ga 69.723
	Zinc 30 Zn 65.38
	Copper 29 Cu 63.546
	Nickel 28 Ni 58.6934
	Cobalt 27 Co 58.9332
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	Manganese 25 Mn 54.938045
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	Vanadium 23 V 50.9415
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	Yttrium 39 Y 88.905848
	Zirconium 40 Zr 91.224
	Niobium 41 Nb 92.90638
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	Osmium 76 Os 190.23
	Iridium 77 Ir 192.222
	Platinum 78 Pt 195.084
	Gold 79 Au 196.966569
	Mercury 80 Hg 200.59
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	Lead 82 Pb 207.2
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	Astatine 85 At [210]
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**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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Prof. Taro Hitosugi (Tohoku University, Tokyo Institute of Technology)

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