

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)

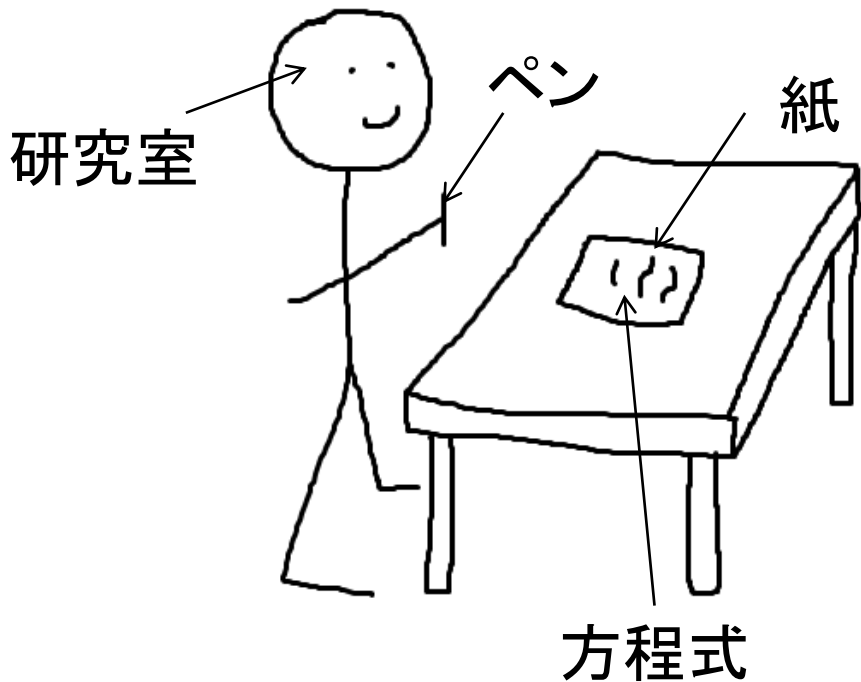
東北大学 原子分子材料科学高等研究機構

科学技術振興機構 さきがけ



東北大学



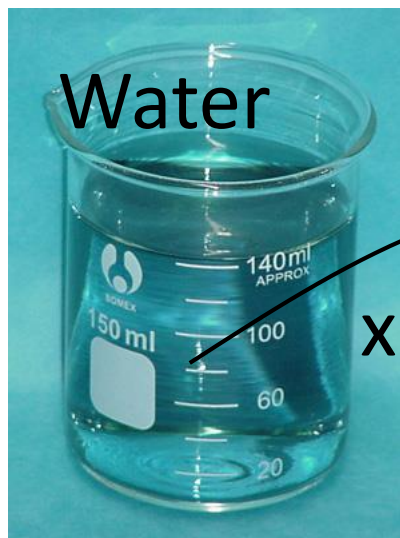


I am a **chemist** and an **applied mathematician**.

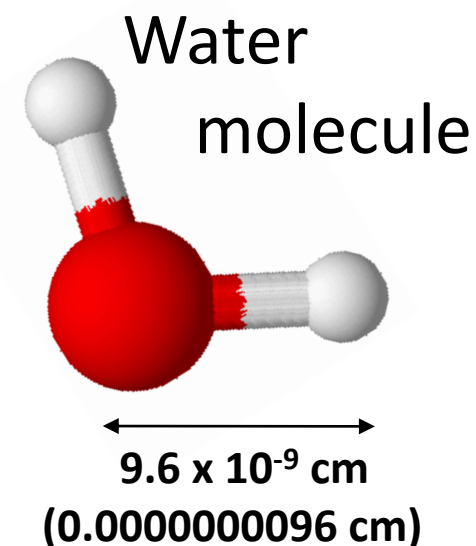
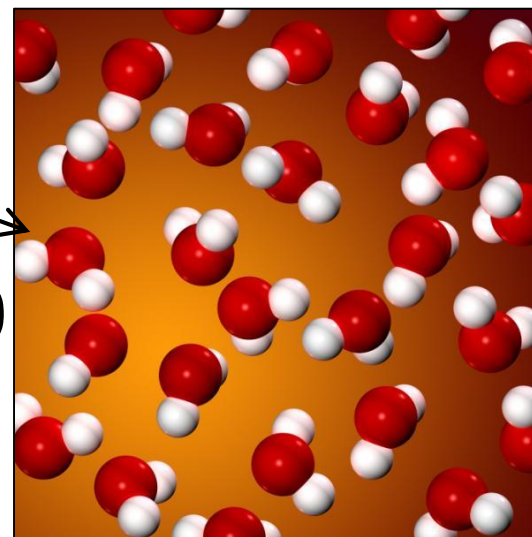
Chemistry = Science of creating new materials using molecules

Applied Mathematics = Science of abstracting natural phenomena

Molecules make up matter

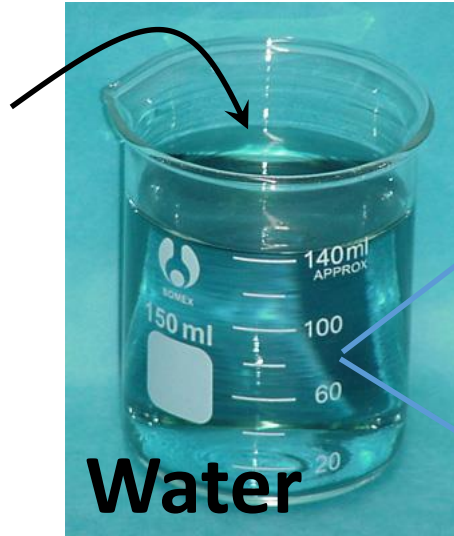
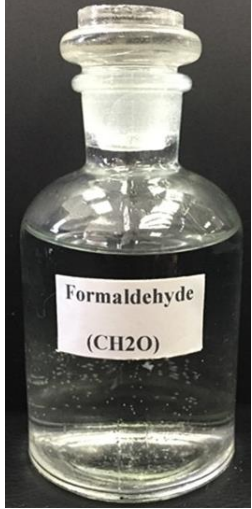


$\times 1000000000000$

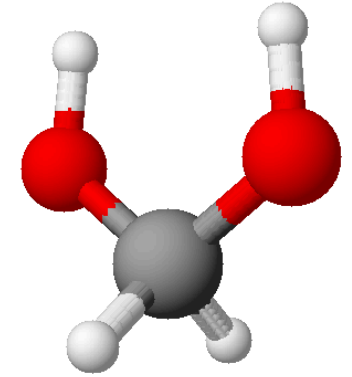
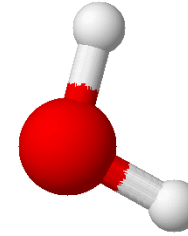
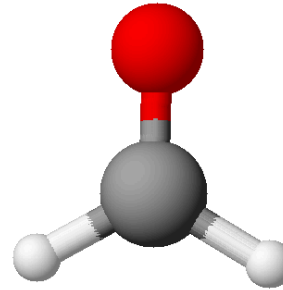


How to make new materials using molecules?

1. Chemists mix molecules together.



2. Molecules **interact** with each other



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

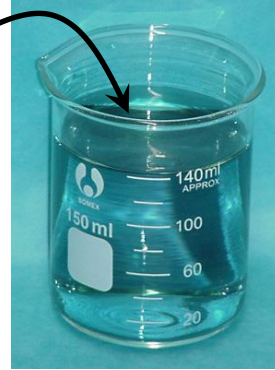
Chemists **can control** this step

Chemists **cannot control** this step!

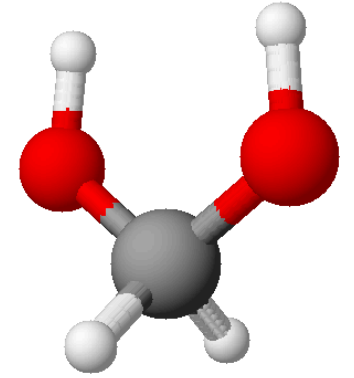
Key point: Before mixing the molecules together, chemists must **know the rules** for how the molecules will interact.

What is a rule?

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



Rule



How to deduce new rules?

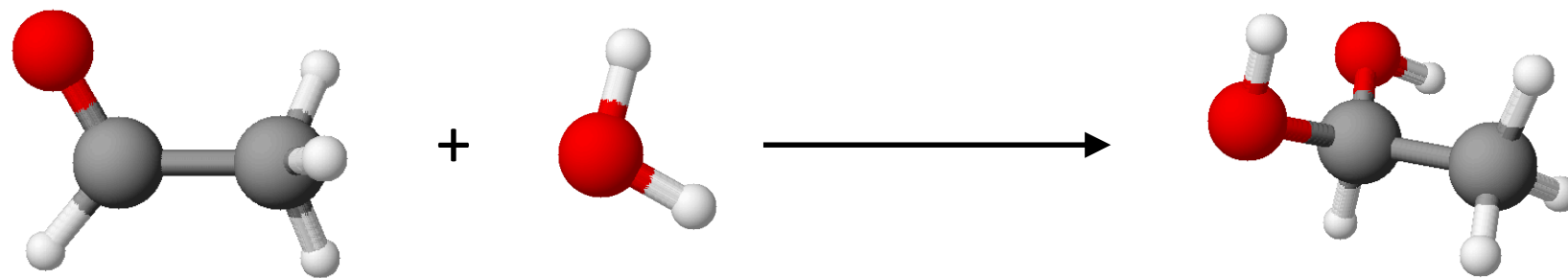
This is very difficult.

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

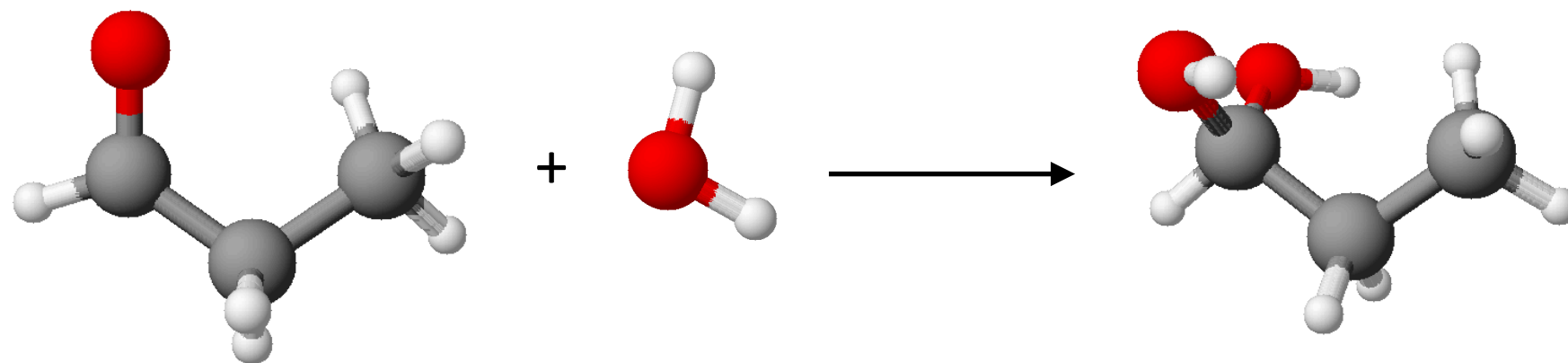


Example: Let's deduce a rule!

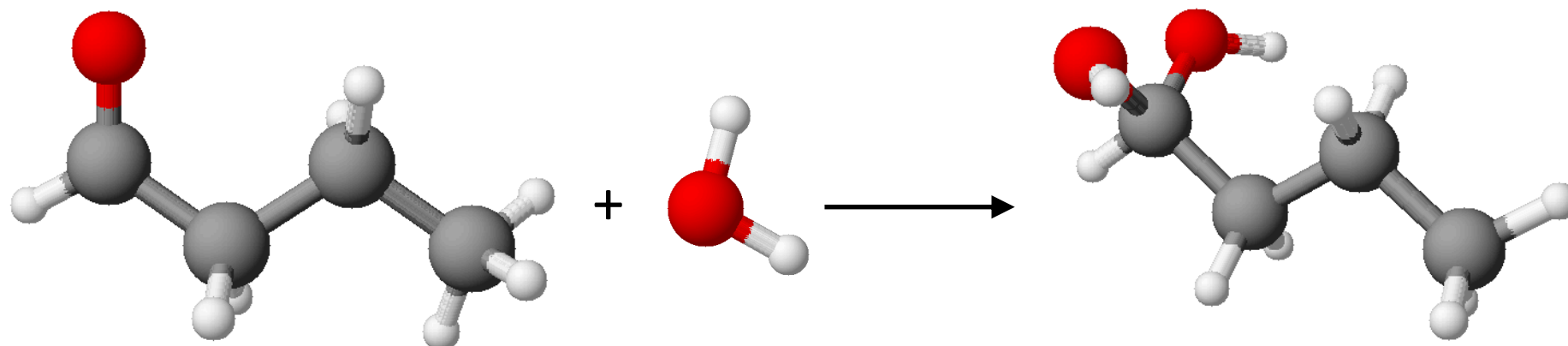
Experiment 1



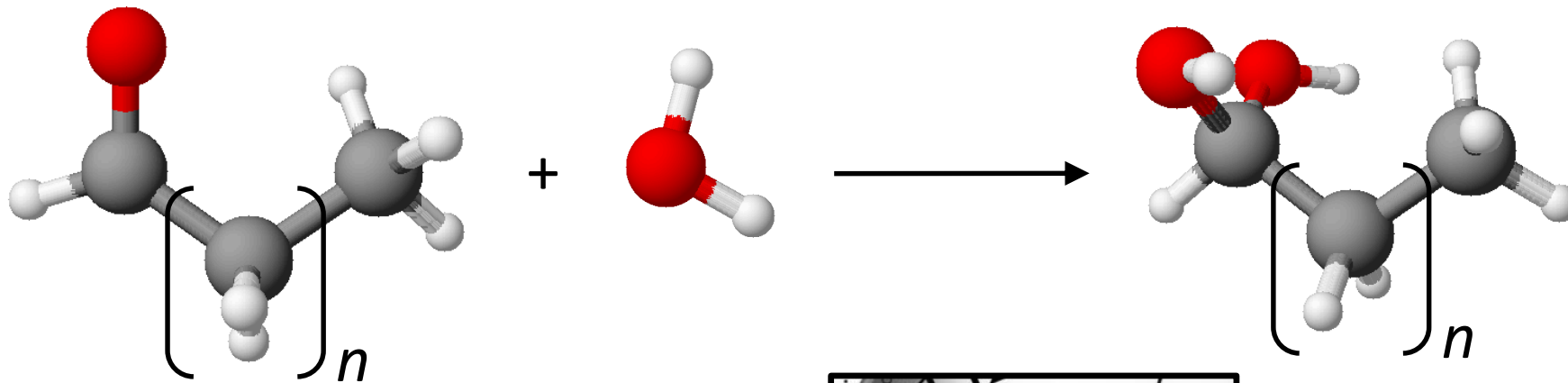
Experiment 2



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:

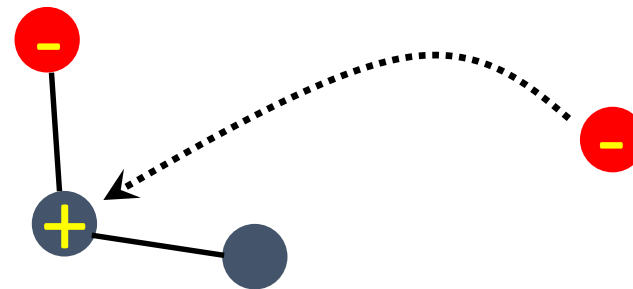
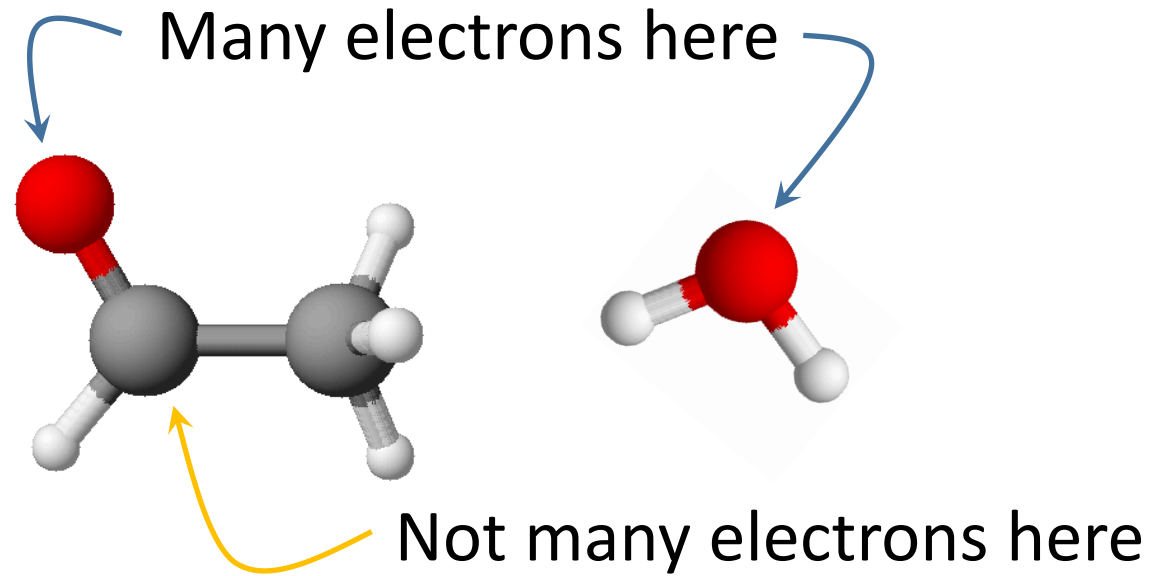
2. **Abstract** the real situation

3. Apply the **laws of physics**

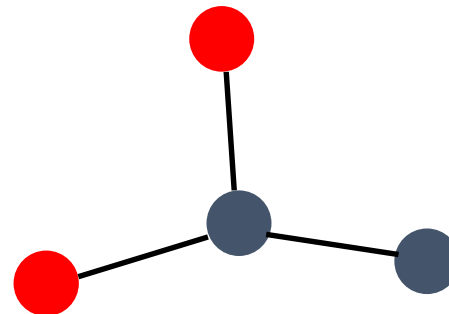
→ Tells us the rule

4. Compare to **experiment**

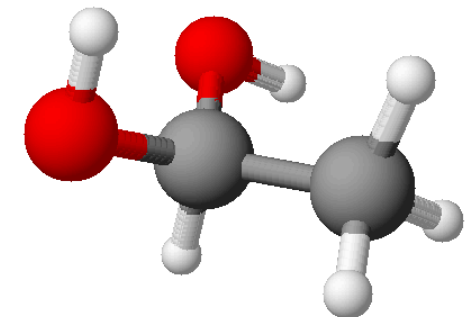
Similar → Rule seems reasonable.



Physics: Positive attracts negative.



Experiment



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!

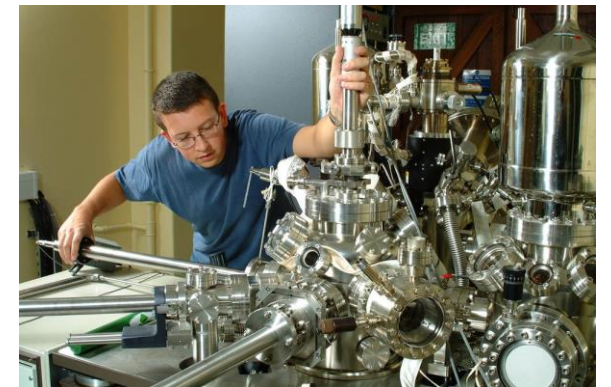
Need friends who can do experiments!

Periodic Table of the Elements

Legend:

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

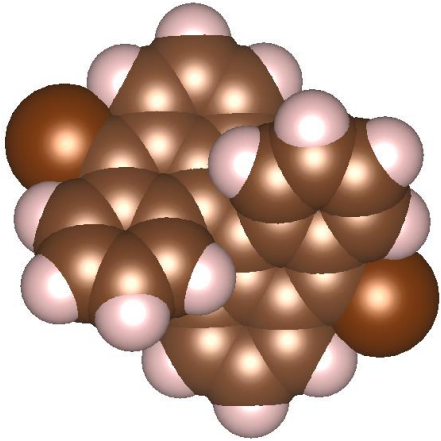
$$\frac{dX_t}{dt} = f(X_t) + b \frac{dW_t}{dt}$$



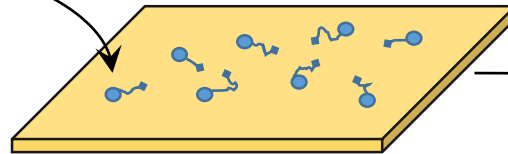
Mathematical modelling for next-generation electrical materials

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

Di-bromo bi-anthryl (DBBA) molecule

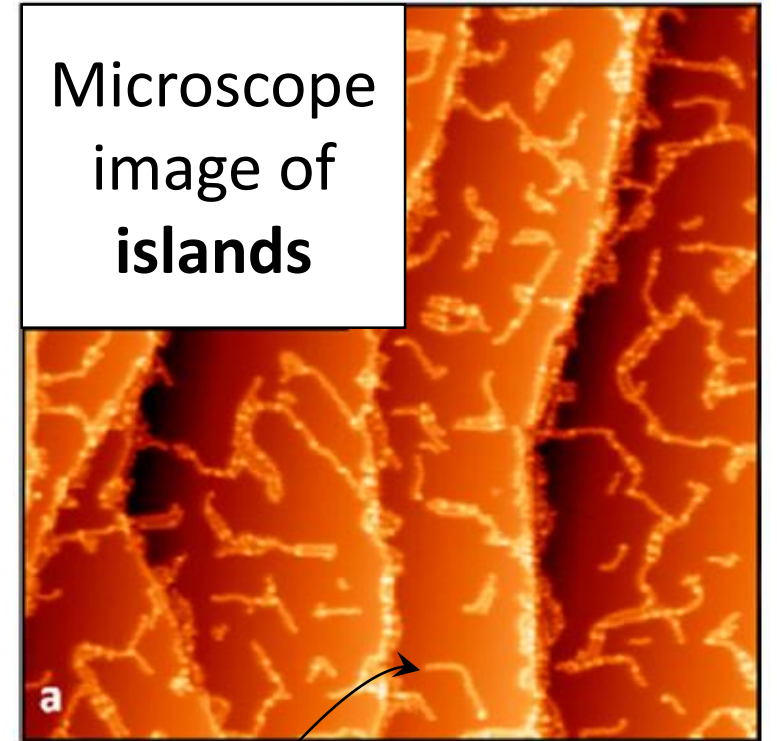


Place on copper surface



Molecules diffuse on surface

← 1.380 x 10⁻⁷m →



↑ 1.380 x 10⁻⁷m ↓

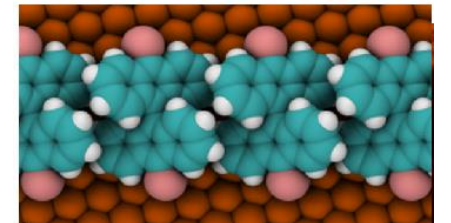
What happened?

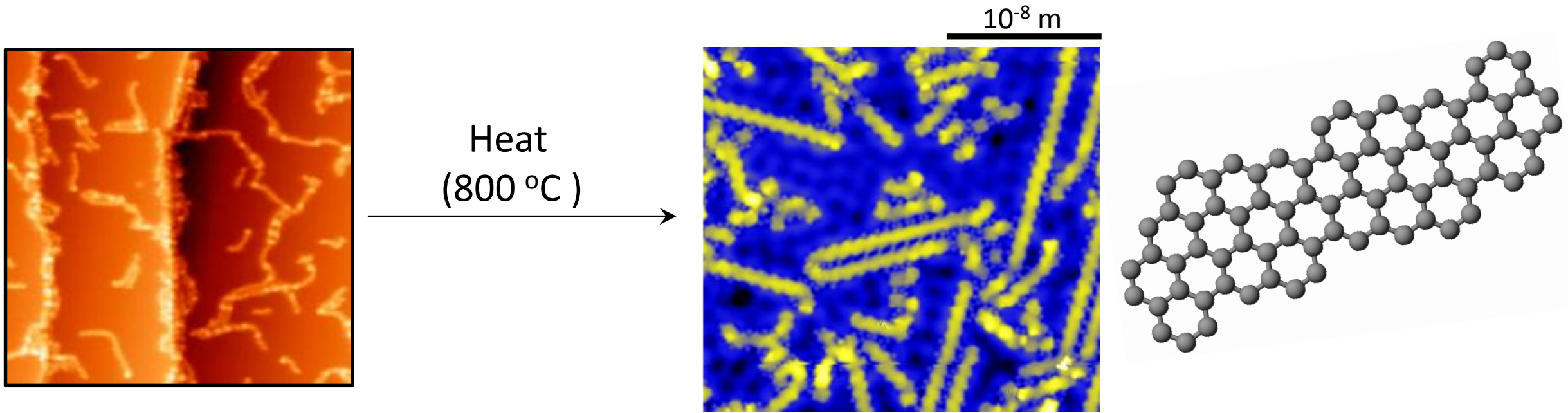
The molecules **assembled into islands**.

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

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

'Molecule island'





Islands turn into **graphene**

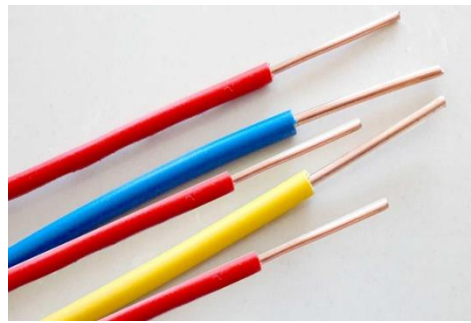
What is special about graphene?

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

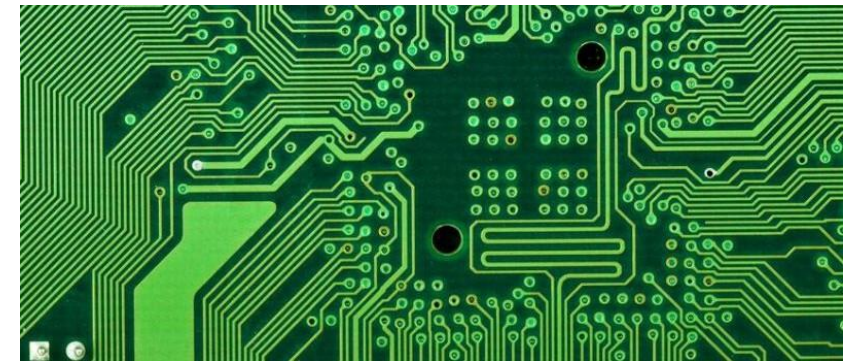
Dream: Create **real electronics** using graphene (e.g., extremely fast computers).

How might we make real electronics using graphene?

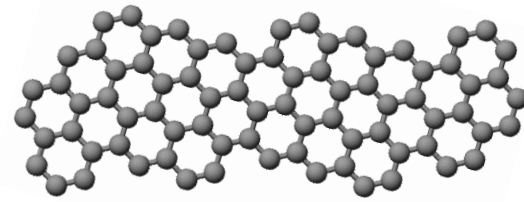
Wire:



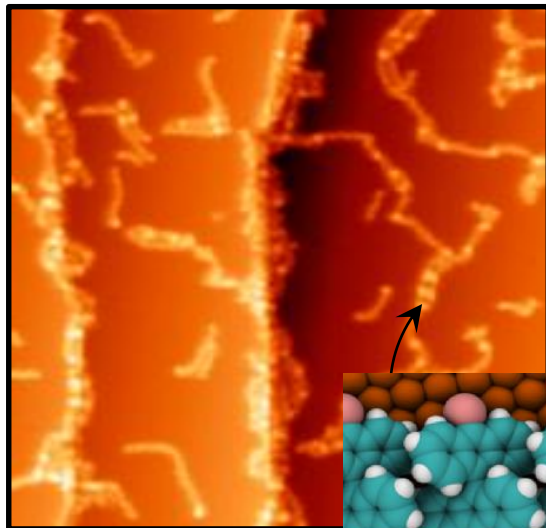
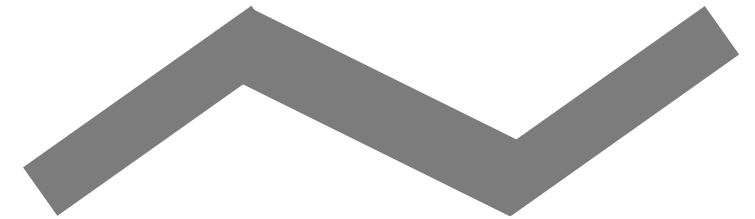
Electronic circuit:



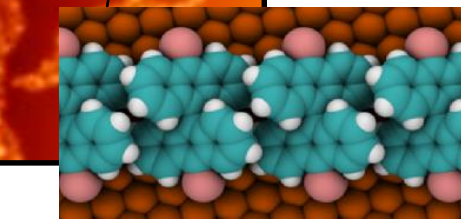
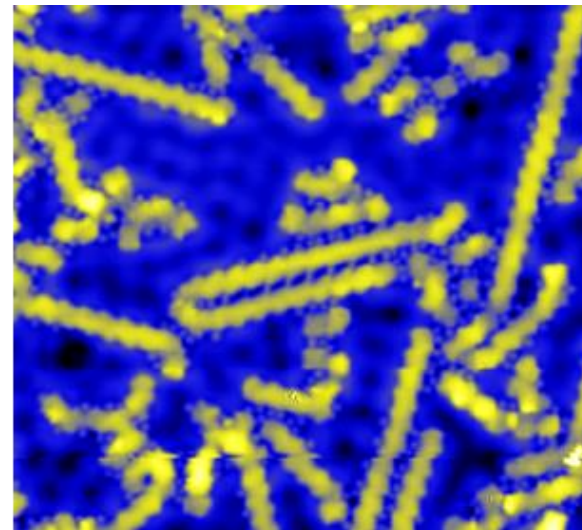
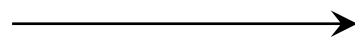
Wire-shaped graphene



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

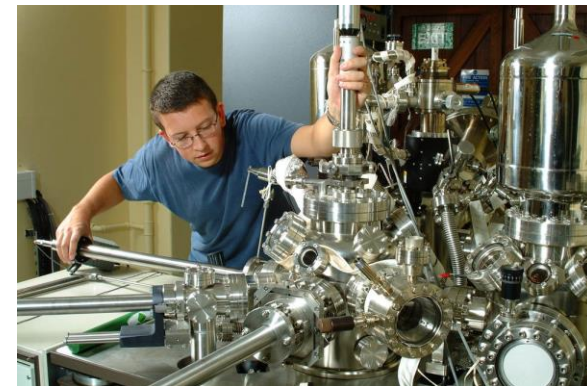
4. Compare to experiment

Periodic Table of the Elements

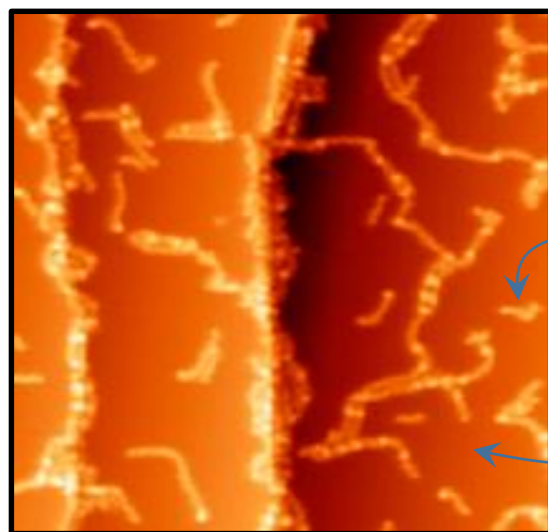
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$$\frac{dX_t}{dt} = f(X_t) + b \frac{dW_t}{dt}$$

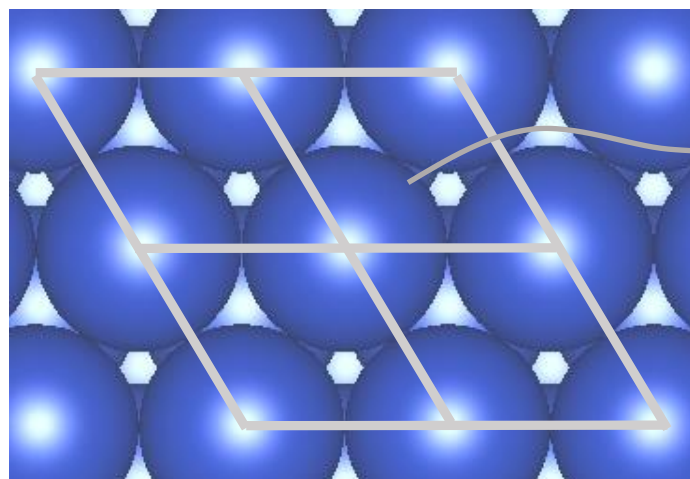
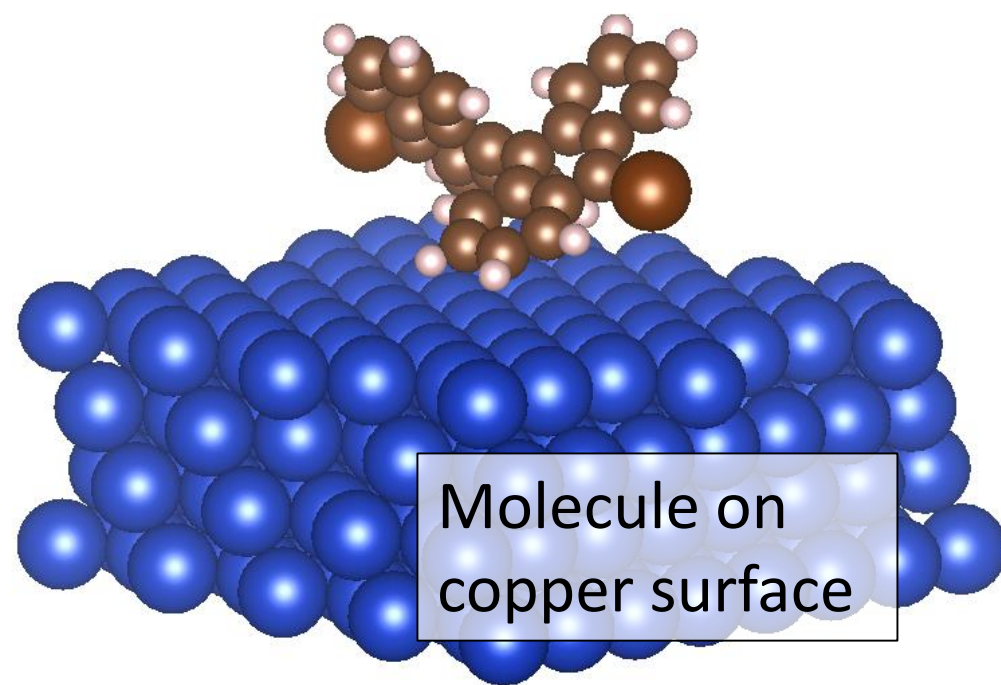


1. Key parts of the real situation

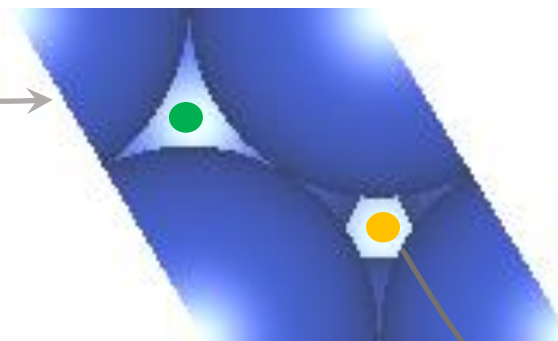


Island made of molecules

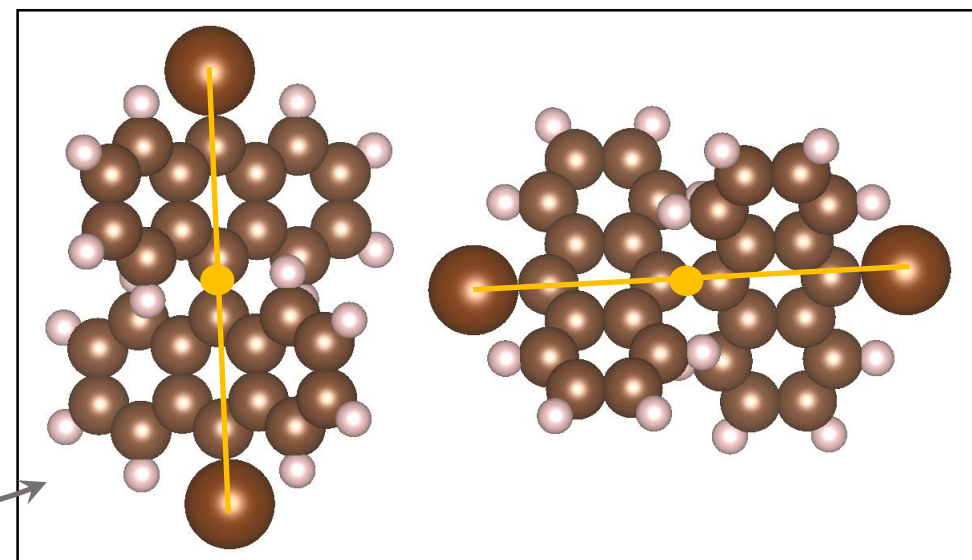
Copper surface



Unit cells of metal surface



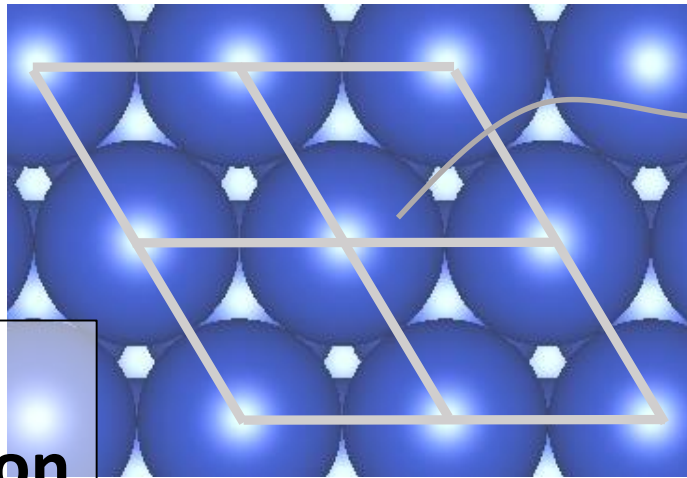
Adsorption sites



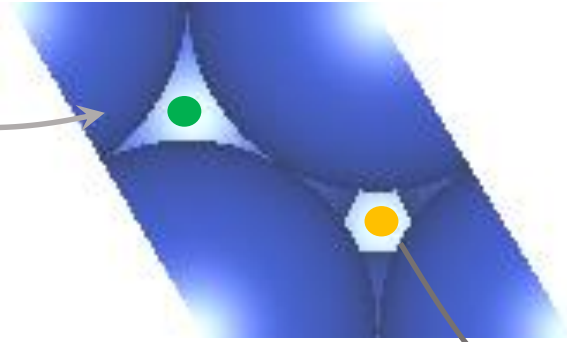
Molecule orientations

2. Abstract the real situation

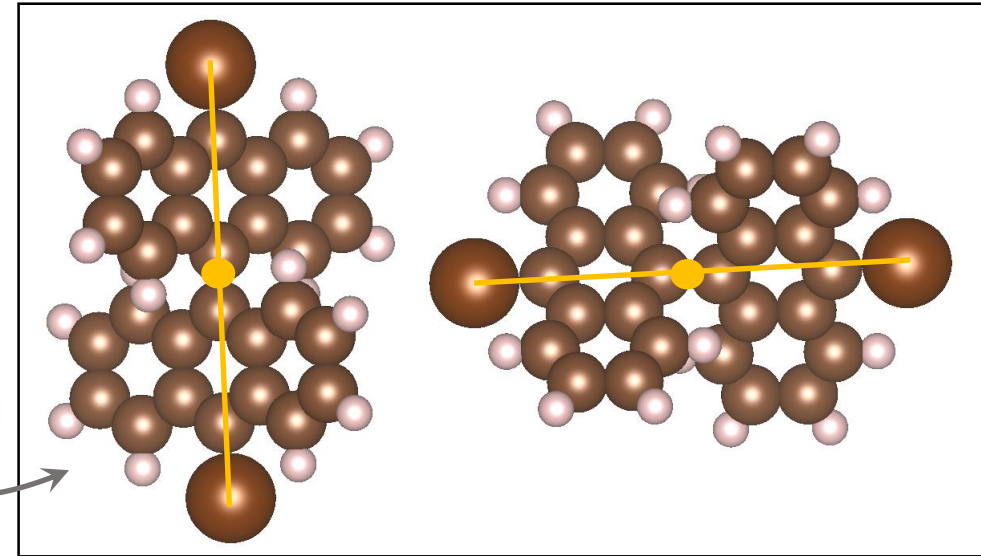
Real situation



Unit cells of metal surface

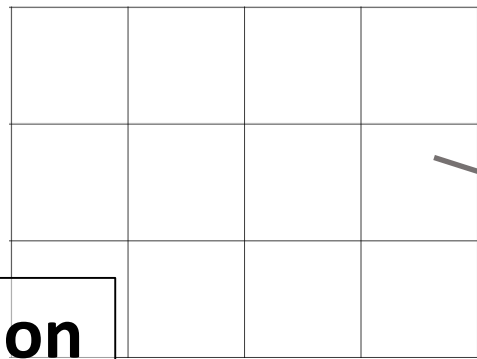


Adsorption sites



Molecule orientations

Abstraction

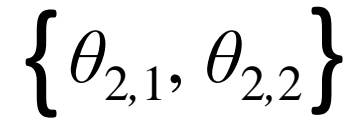


'Cells' C_1, C_2, \dots, C_M



'Colours'

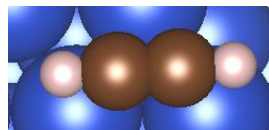
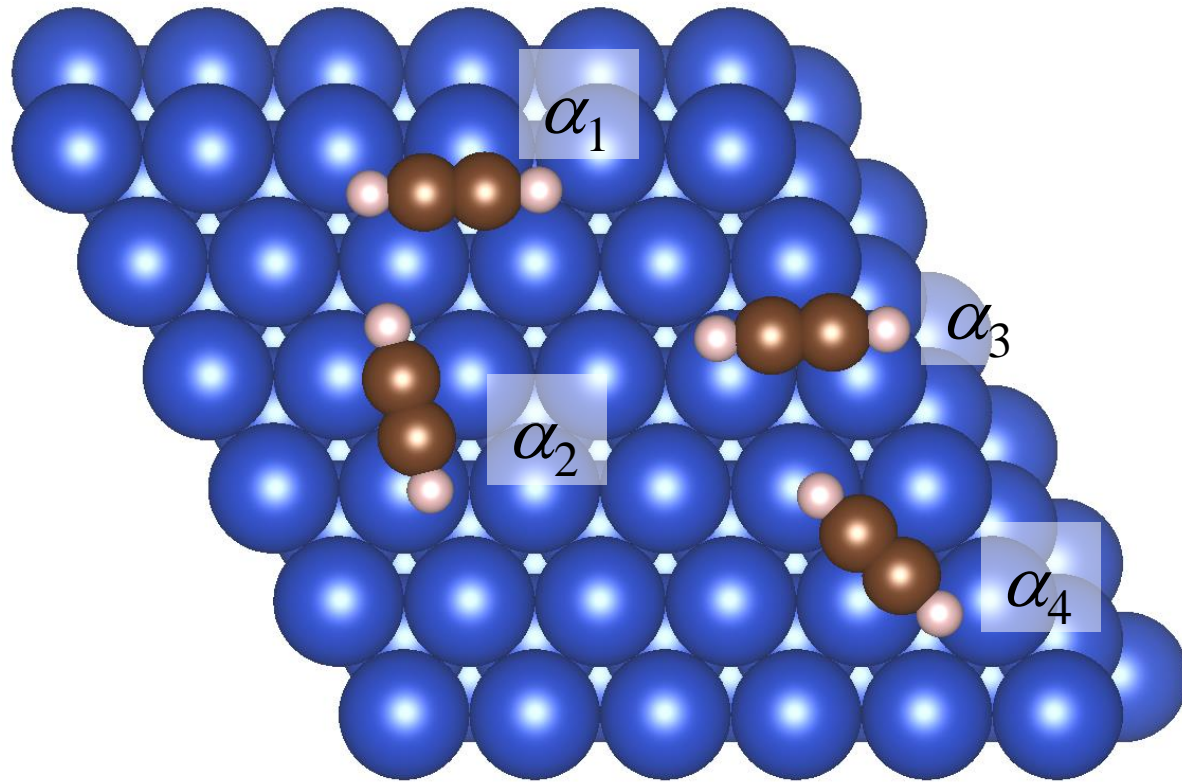
$\sigma_1, \sigma_2, \dots, \sigma_k$



'Shades'

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

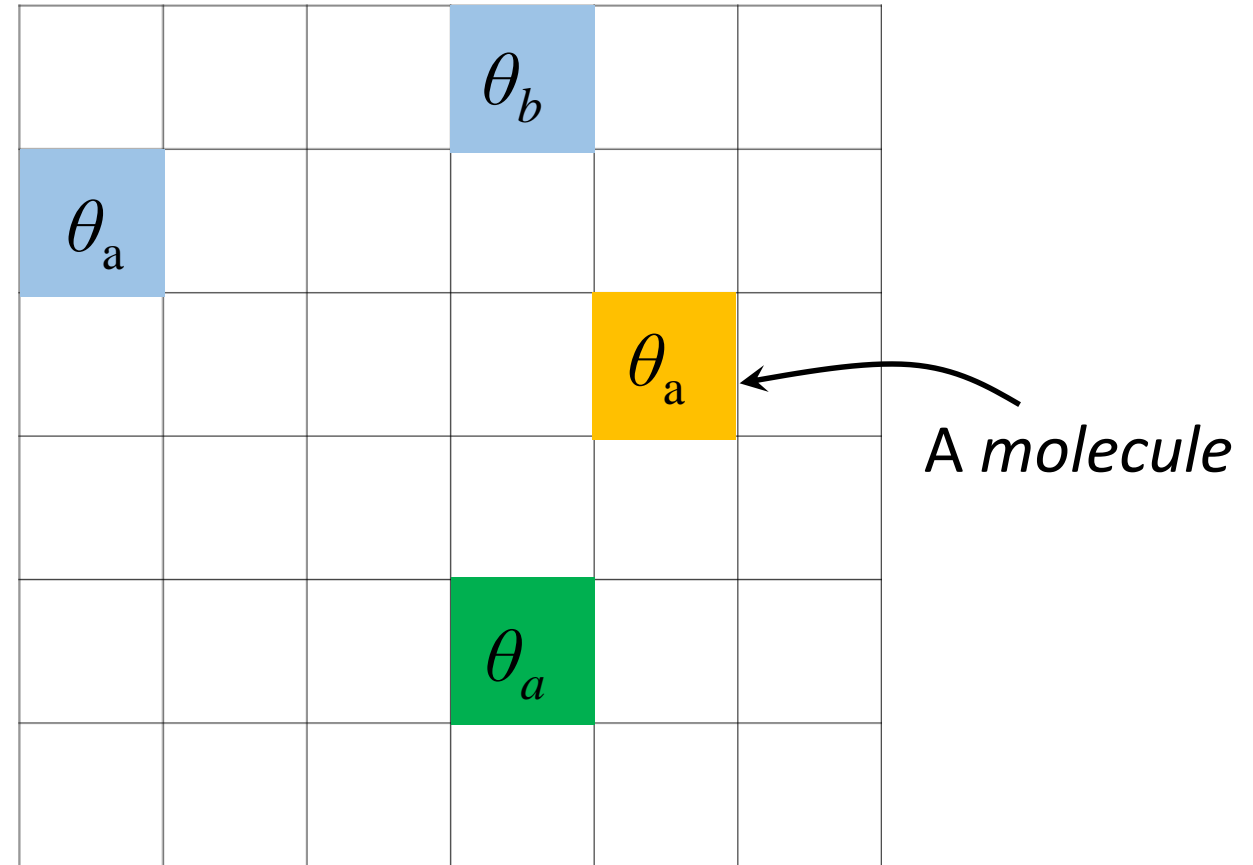
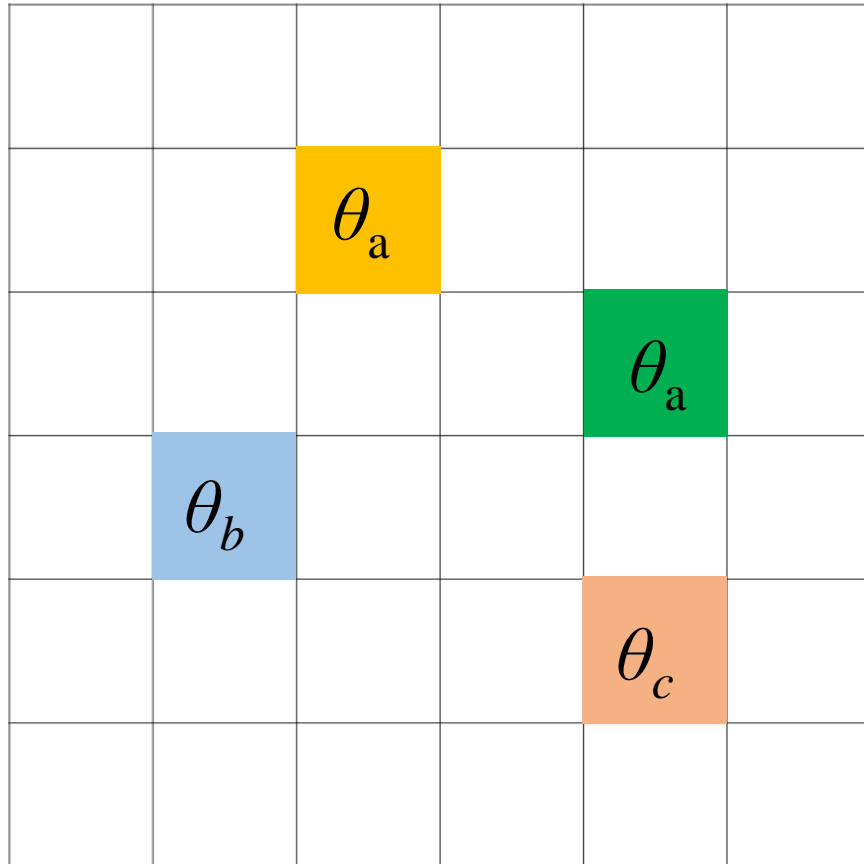
Reality – abstraction correspondence



= HCCH molecule

		θ_a	α_1		
				θ_a	α_3
	θ_b	α_2			
				θ_c	α_4

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



Two configurations ($N = 4$, four colors ● ● ● ●, 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

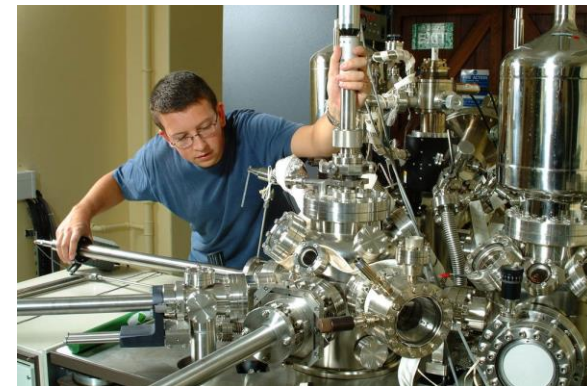
Legend:

- Alkali Metal
- Alkaline Earth
- Transition Metal
- Basic Metal
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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

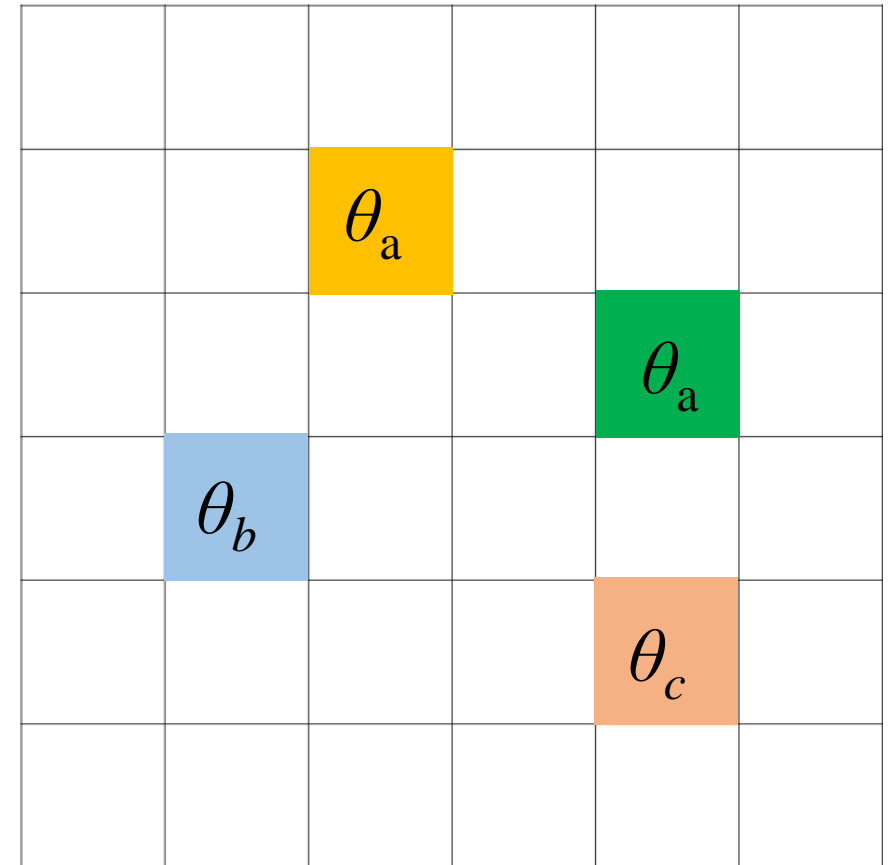
→ probability of configuration c

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

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

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

T = Temperature

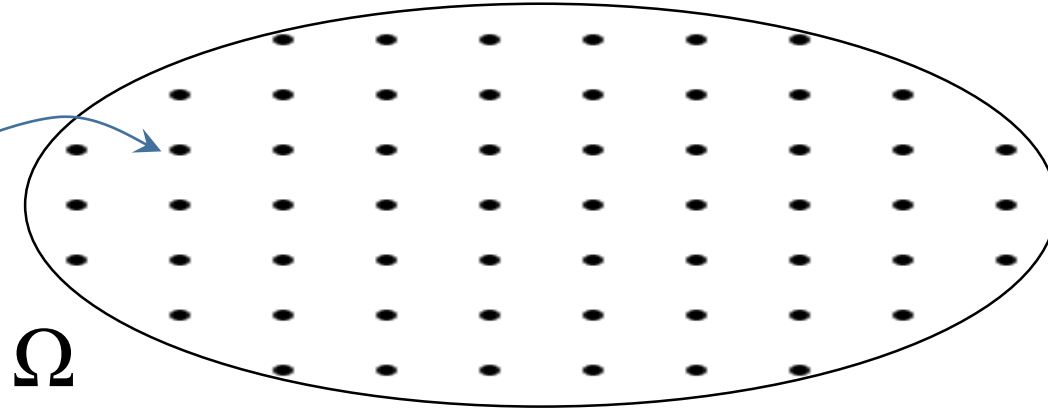
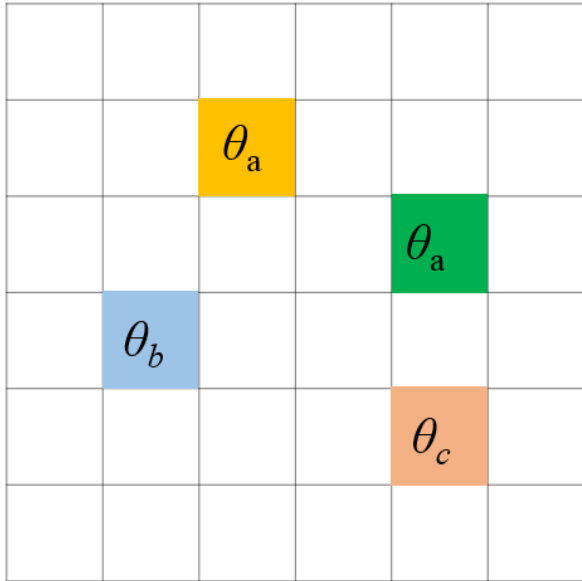


one configuration (c)

Mathematical challenge

Find configurations that have high probability.

Search for High Probability Configurations



Ω = configuration space

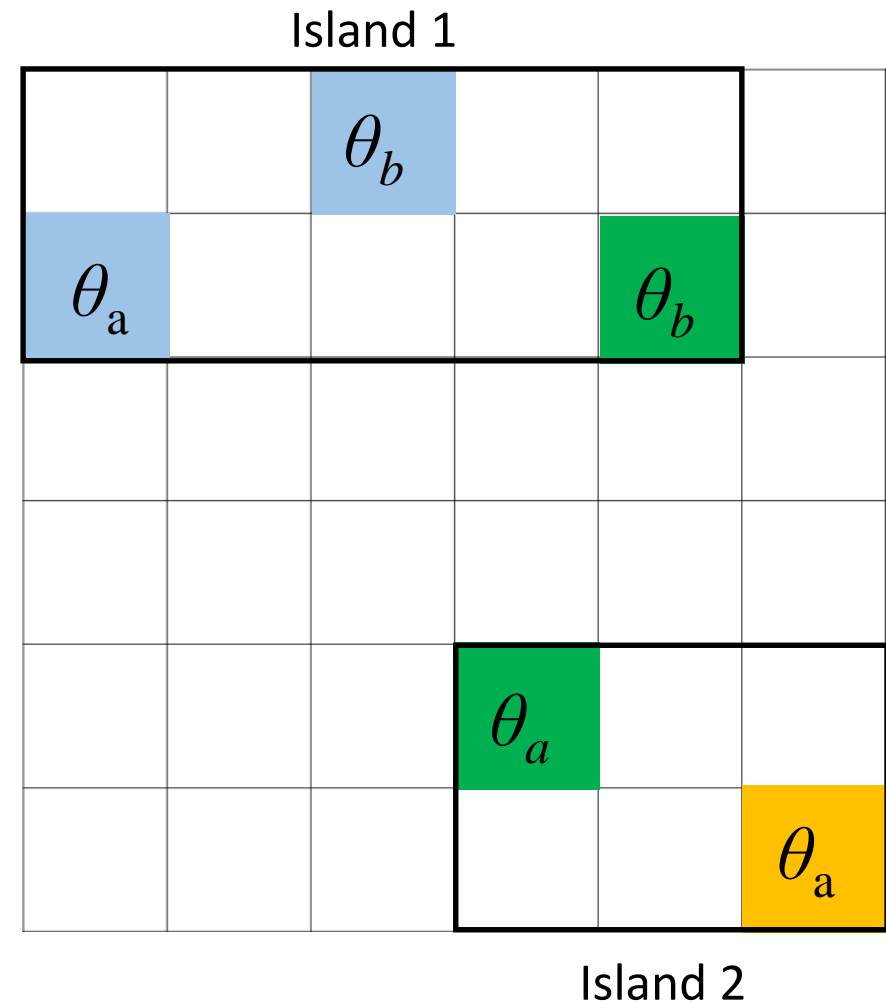
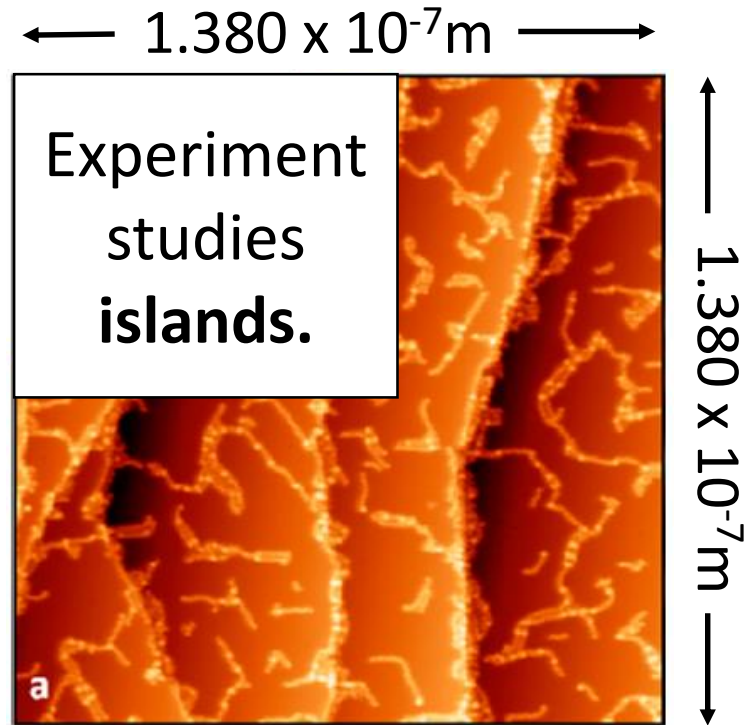
Configuration space is extremely big!

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.

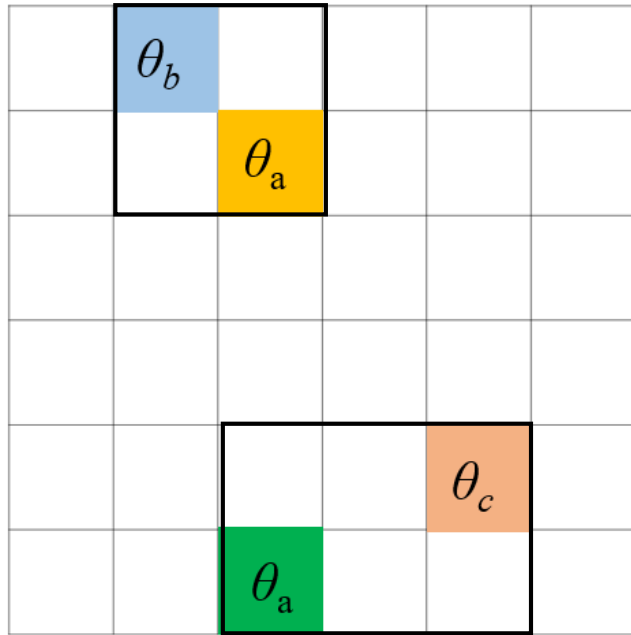
Then $10^{23} \times 10^{-6}$ s $\approx 10^{10}$ years to check probability for every configuration!

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

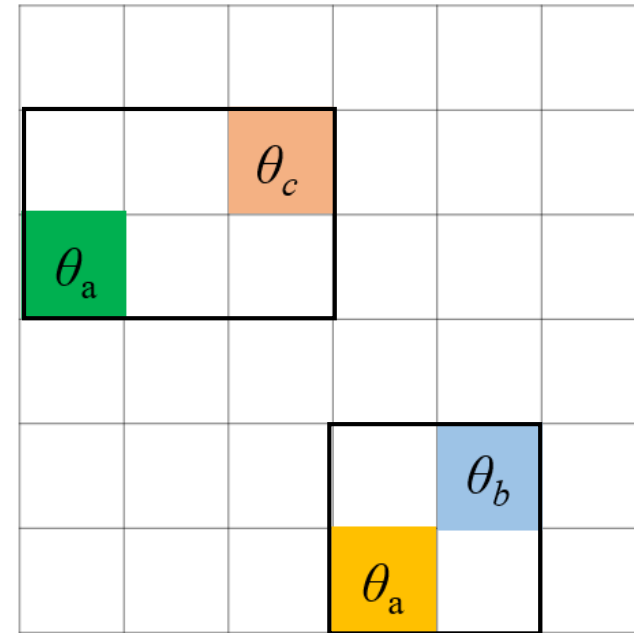
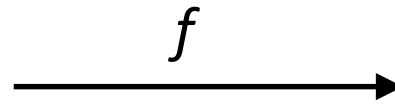


Mathematical definition of **islands**?

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**.

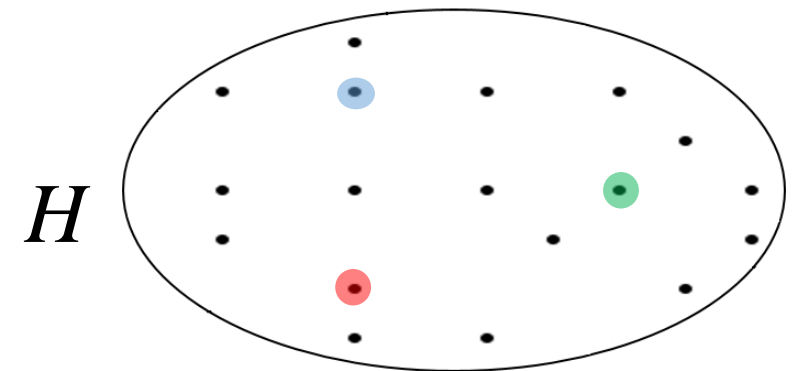
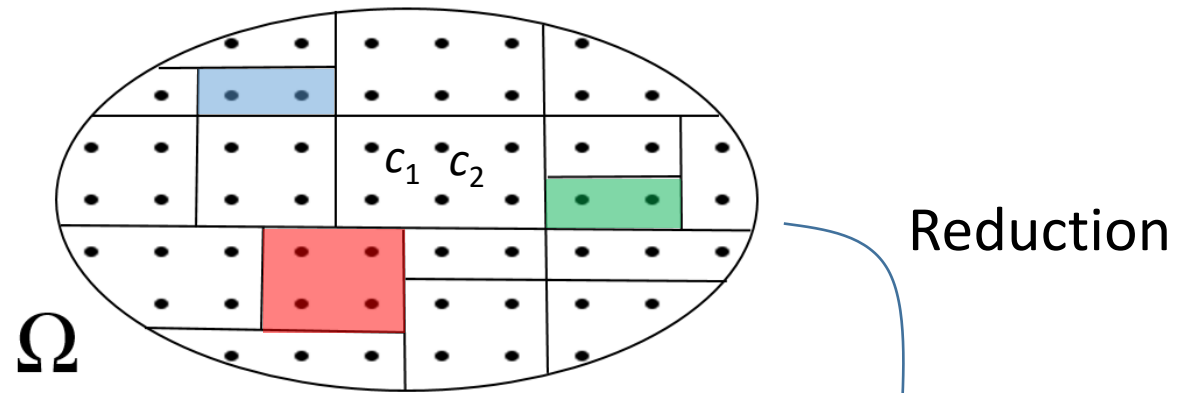
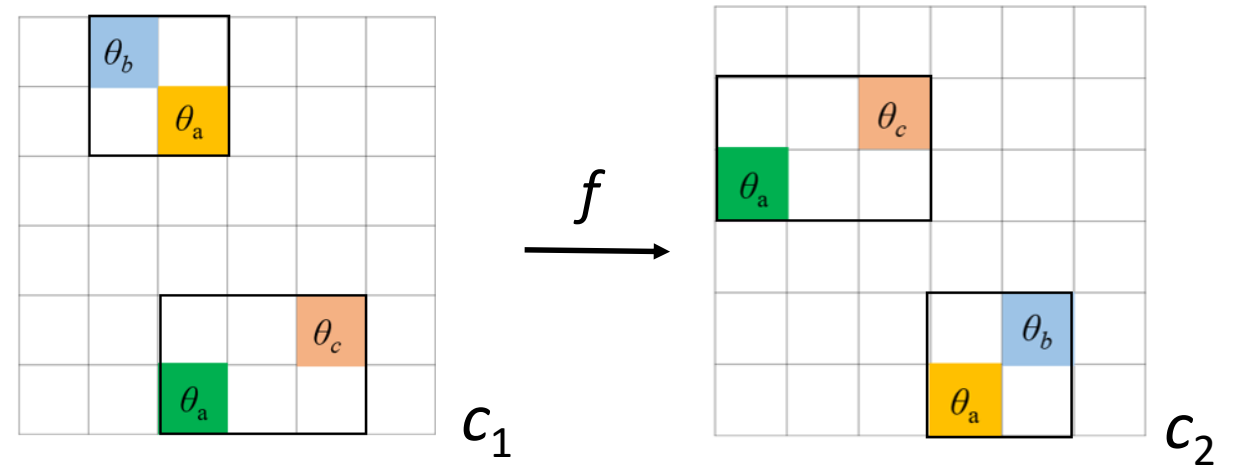
The isomorphism divides the configuration space into **equivalence classes**

Reduced space H
= collection of equivalence classes

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

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

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



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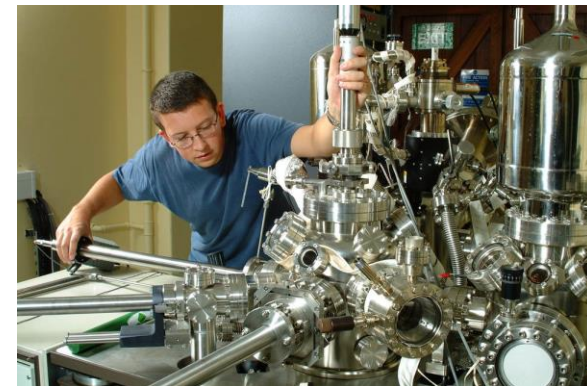
Periodic Table of the Elements

1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
IA	IIA	IIIB	IVB	VB	VIB	VIB	VIII	VIII	VIII	IB	IIB	IIIA	IVA	VVA	VIA	VIIA	VIIIA
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 Bohrium [264]	108 Hs Hassium [265]	109 Mt Meitnerium [268]	110 Ds Darmstadtium [271]	111 Rg Roentgenium [272]	112 Cn Copernicium [285]	113 Nh Nihonium [284]	114 Fl Flerovium [289]	115 Uup Ununpentium [288]	116 Lv Livermorium [293]	117 Uus Ununseptium [294]	118 Uuo Ununoctium [294]

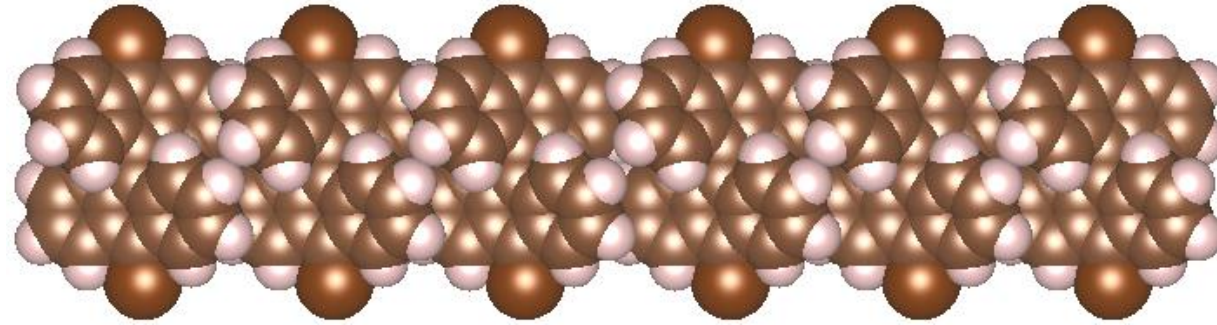
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- Semimetal
- Nonmetal
- Halogen
- Noble Gas
- Lanthanide
- Actinide

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

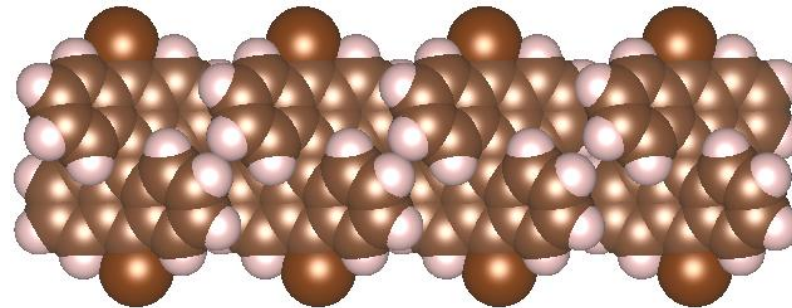


Mathematical
modelling (-123°C)



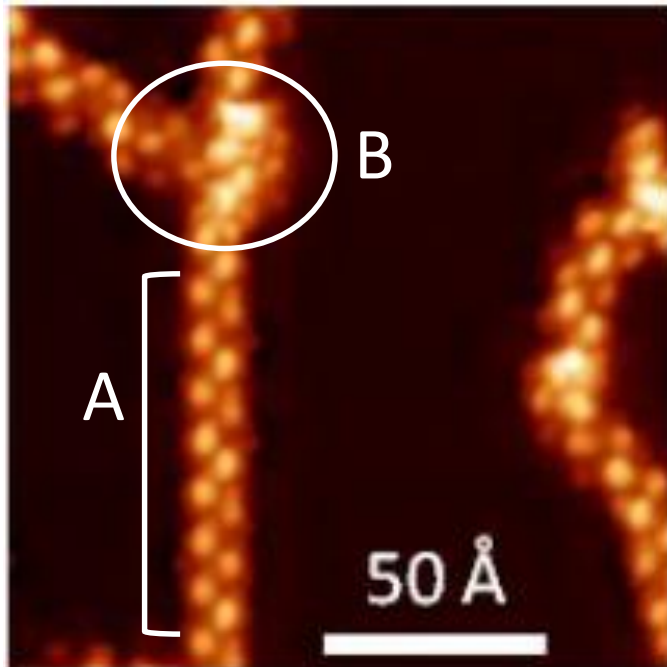
Island 1

+



Island 2

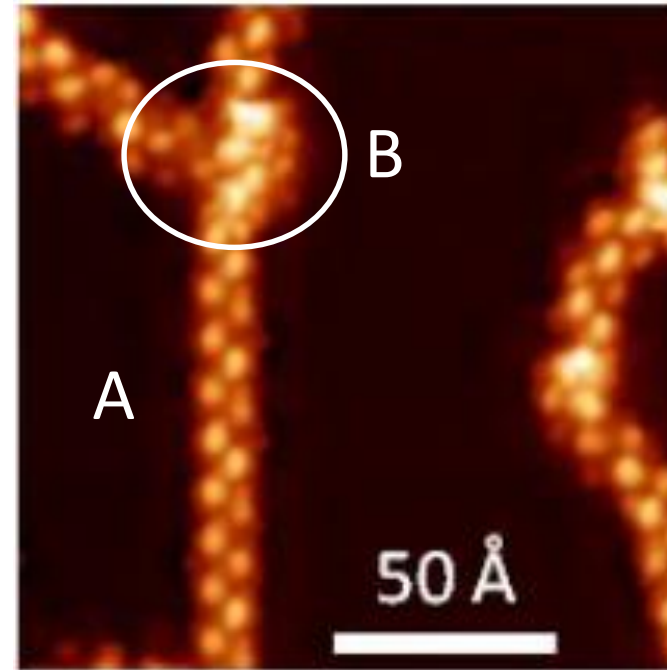
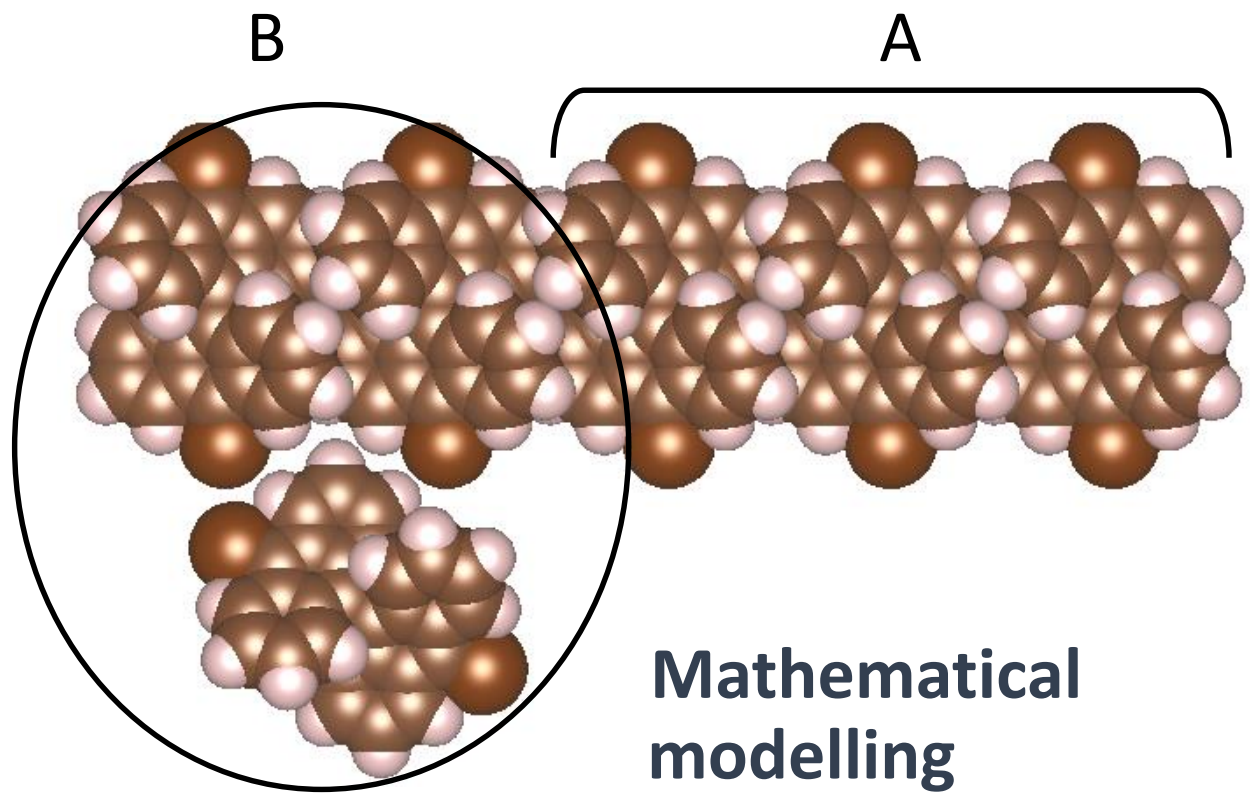
Experiment (30°C)



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

But: What about the part in (B)?

Let's consider a higher temperature...

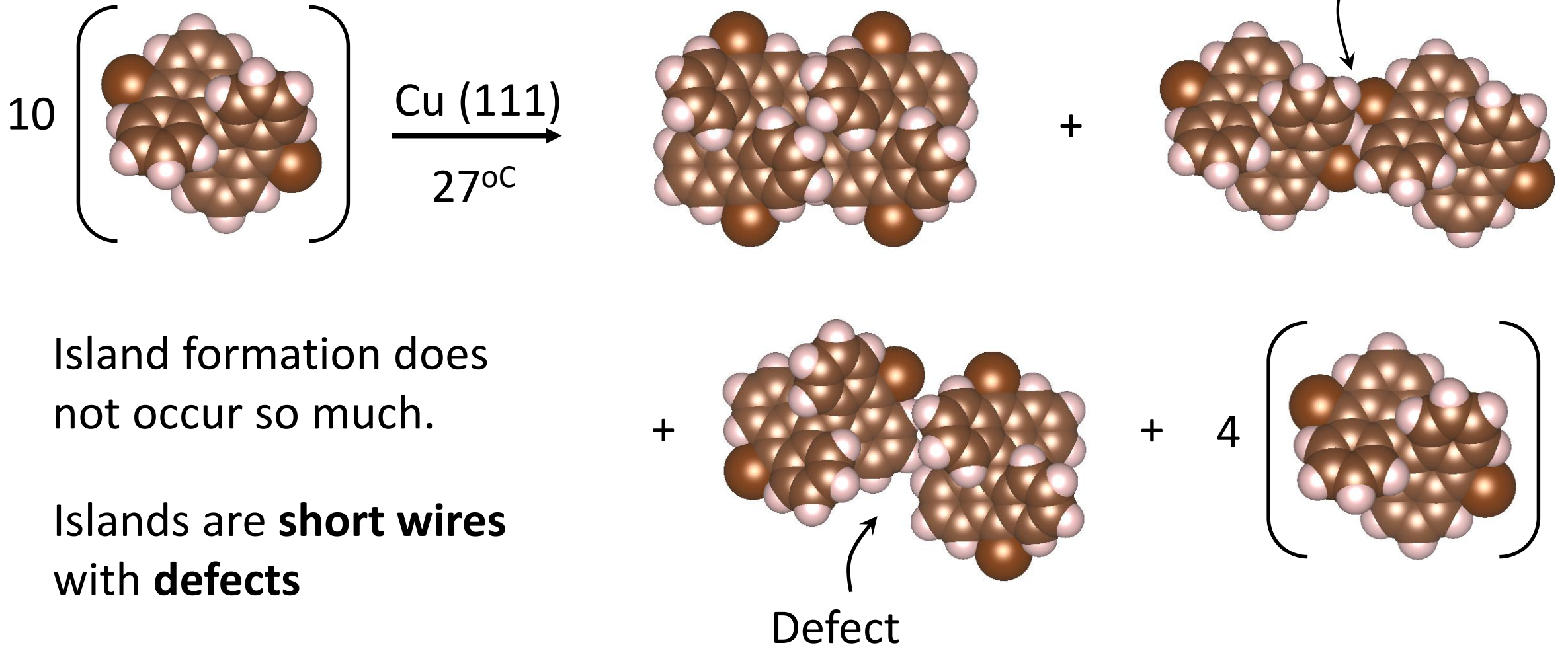


Experiment

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

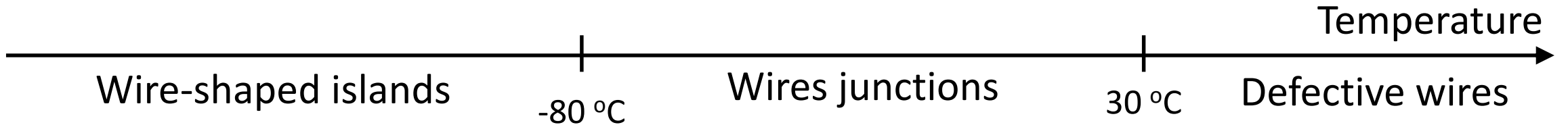
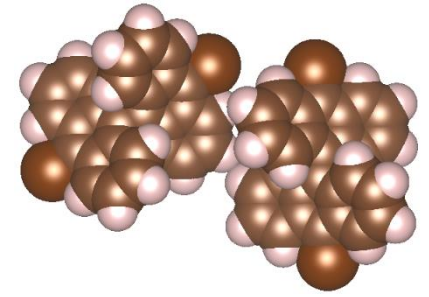
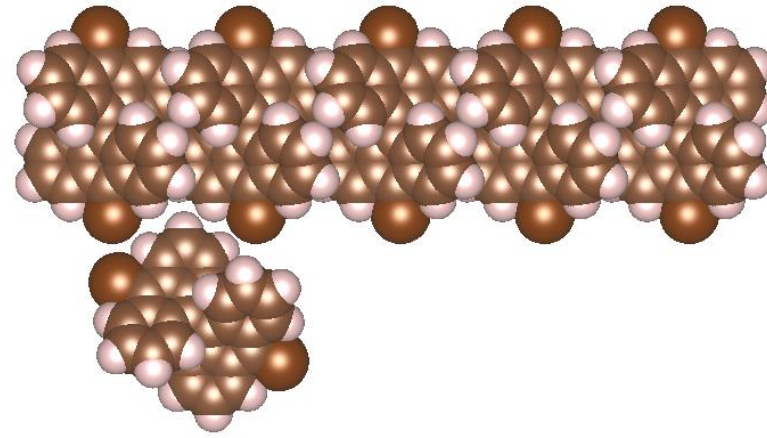
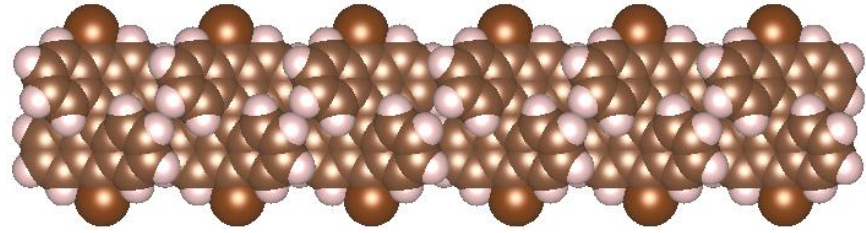
What about even higher temperatures?

High probability islands



Now, the rule starts to appear....

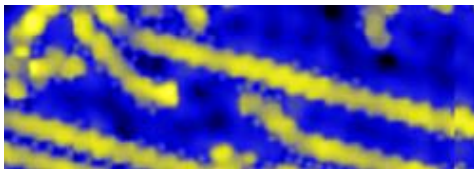
Rules for island formation and graphene production



Heat



10^{-8} m



Graphene wires

Heat



10^{-8} m



Graphene wires with junctions

Heat




Low-quality
graphene wires

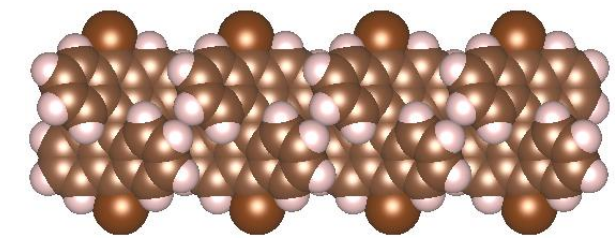
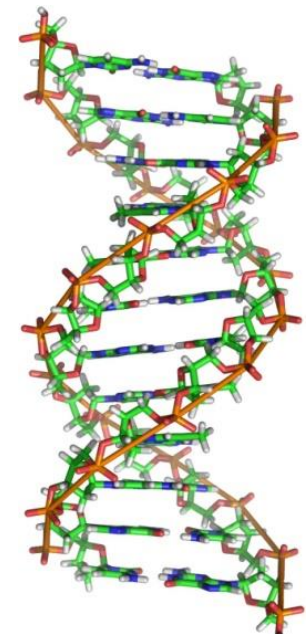
Progress of chemistry

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]
* Lanthanide series	
** Actinide series	



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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