

第1部 各分野におけるデザインとそのプロセス  
Materials and Energy  
マテリアル・エネルギー

Carbon nanotube

Boron nitride  
nanotube

MoS<sub>2</sub> nanotube

● N ● S  
● C ● B ● Mo

R. Xiang et al., *Science* **367** (2020) 537.

Shigeo Maruyama (丸山 茂夫)

School of Engineering, The University of Tokyo (東京大学 大学院工学系研究科)

# Design?

**Materials**

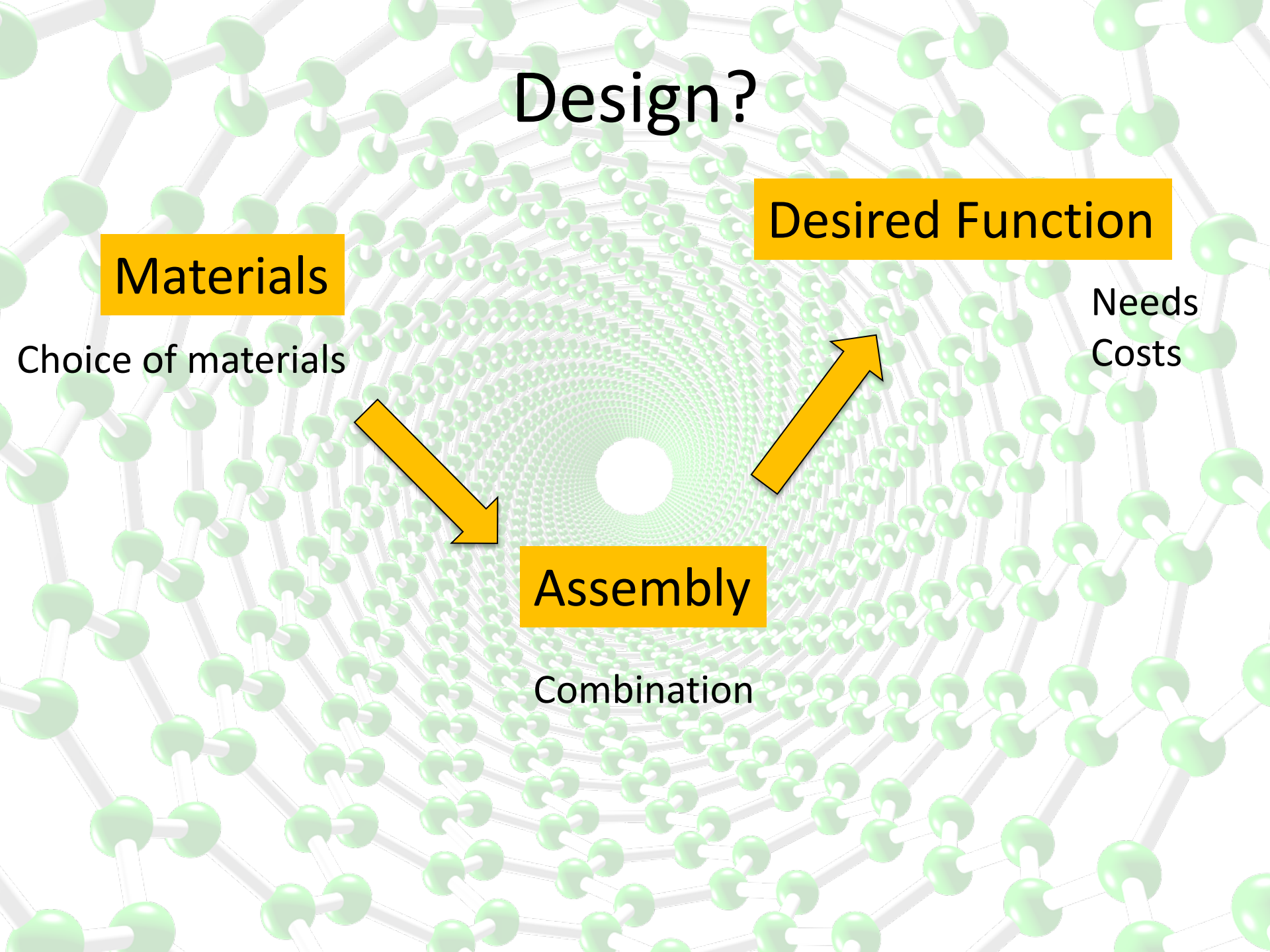
Choice of materials

**Desired Function**

Needs  
Costs

**Assembly**

Combination



# Design?

**Materials**

Choice of materials

**Desired Function**

Needs  
Costs

**Assembly**

Feed back

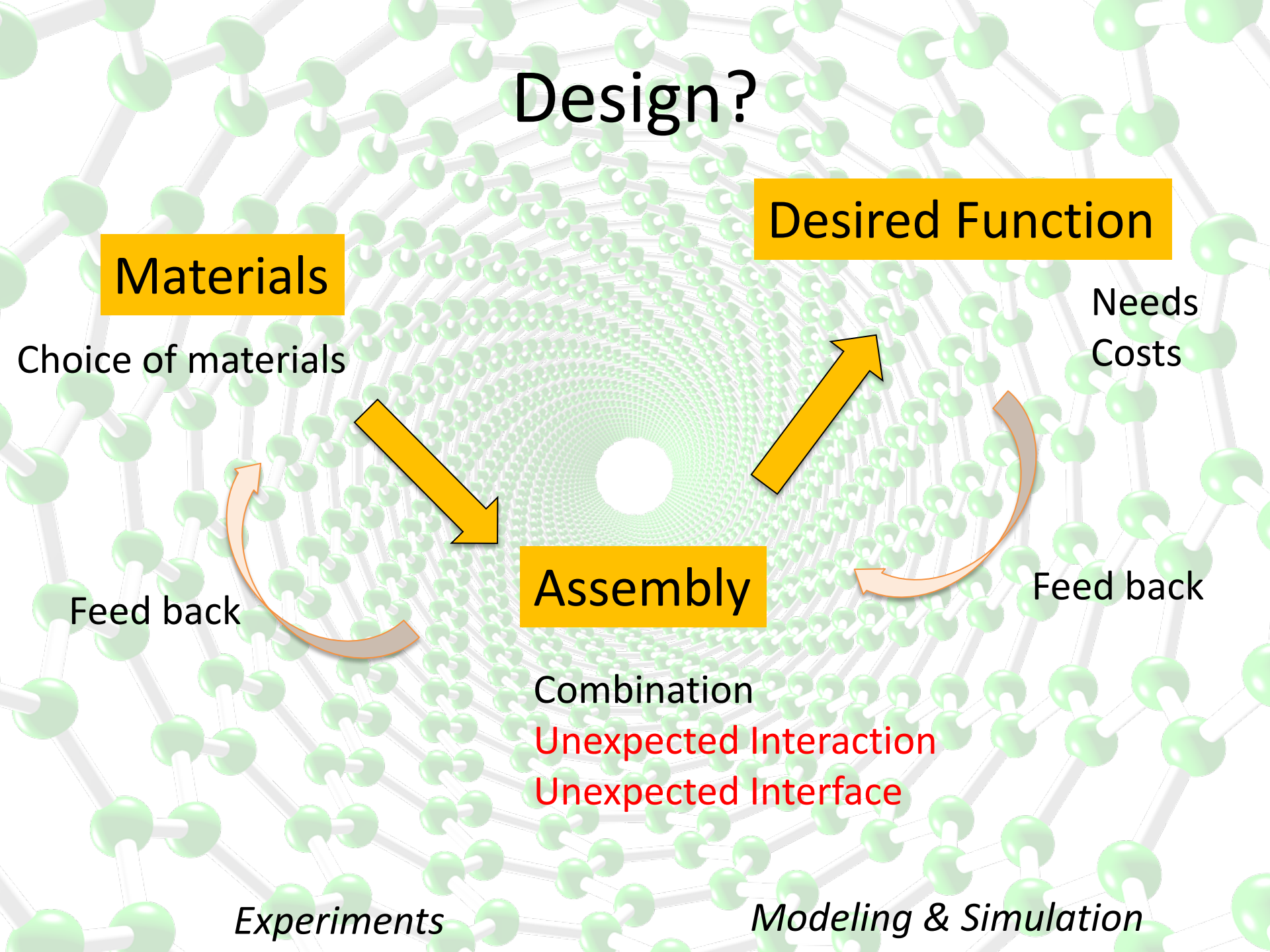
Feed back

Combination

Unexpected Interaction  
Unexpected Interface

*Experiments*

*Modeling & Simulation*

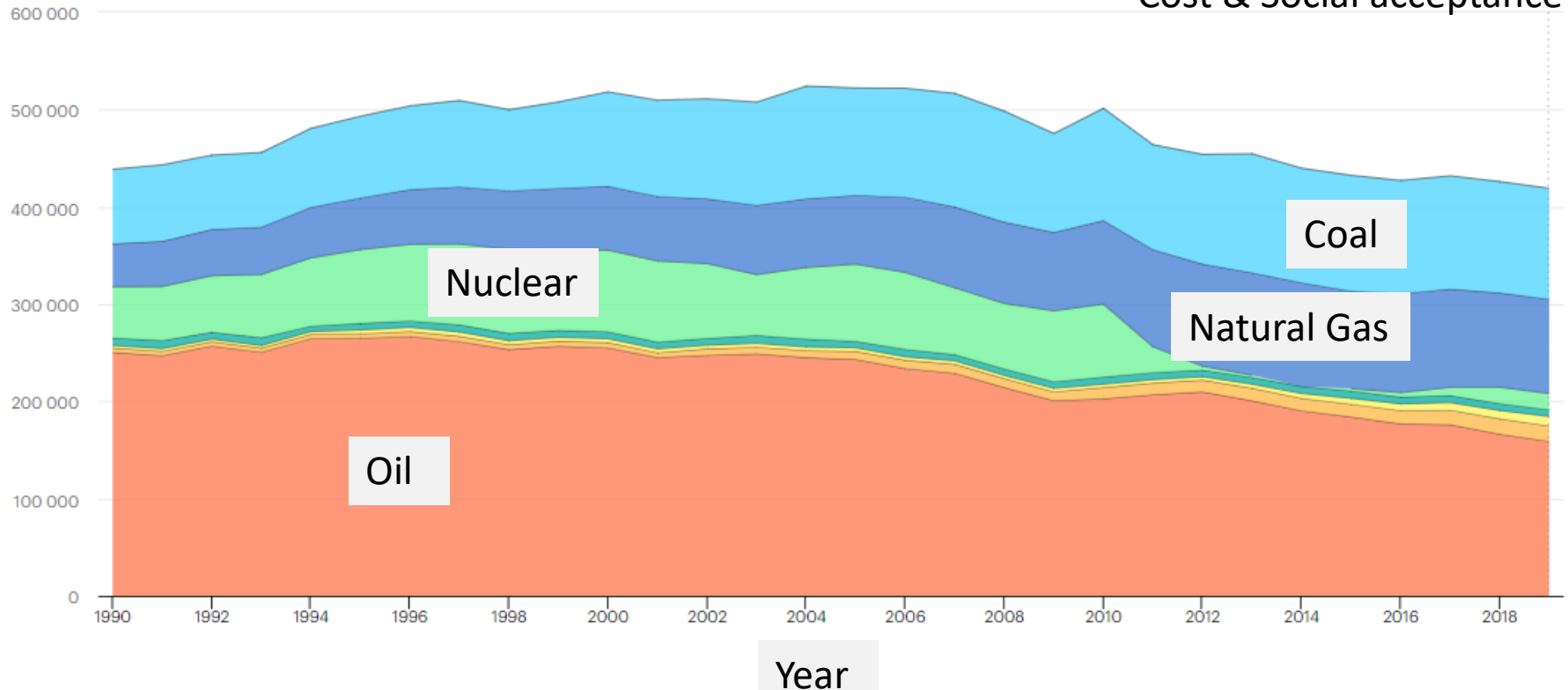


# Energy Sources in Japan

Full of topics of SDGs

- Sustainable Growth
- Global security
- Environmental Issue
- Cost & Social acceptance

ktoe

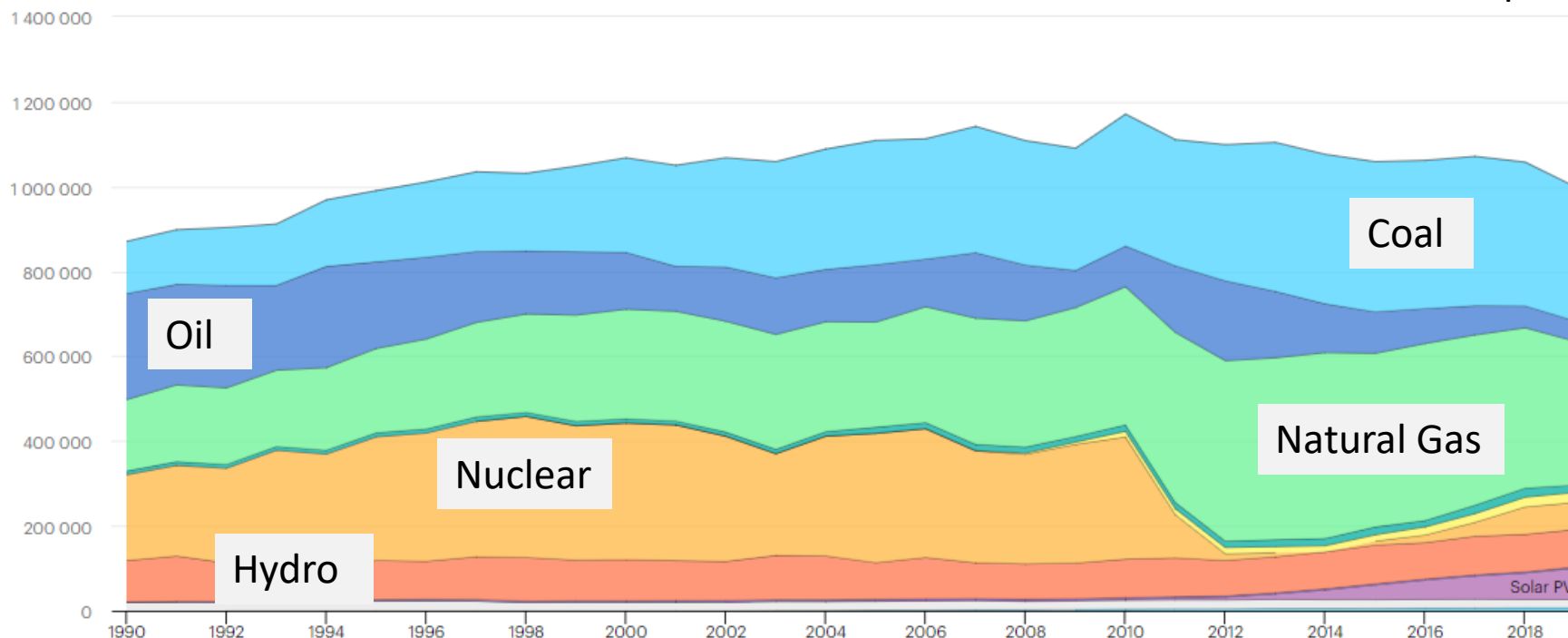


# Electricity Generation in Japan

Full of topics of SDGs

- Sustainable Growth
- Global security
- Environmental Issue
- Cost & Social acceptance

GWh



Year

# Global Energy System

## Materials

Choice of Energy Sources  
Oil, Coal, Natural Gas  
Nuclear, Renewable

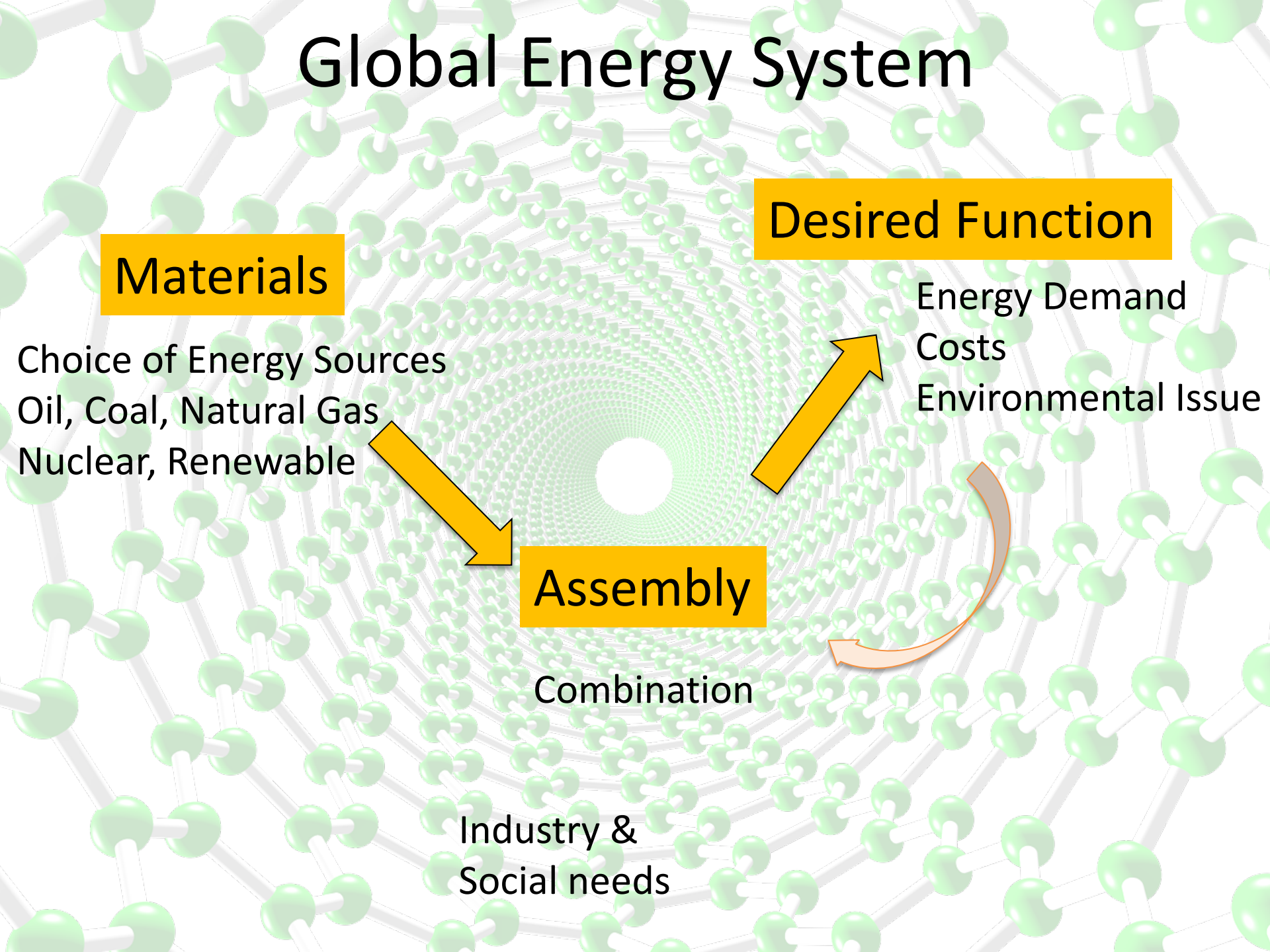
## Desired Function

Energy Demand  
Costs  
Environmental Issue

## Assembly

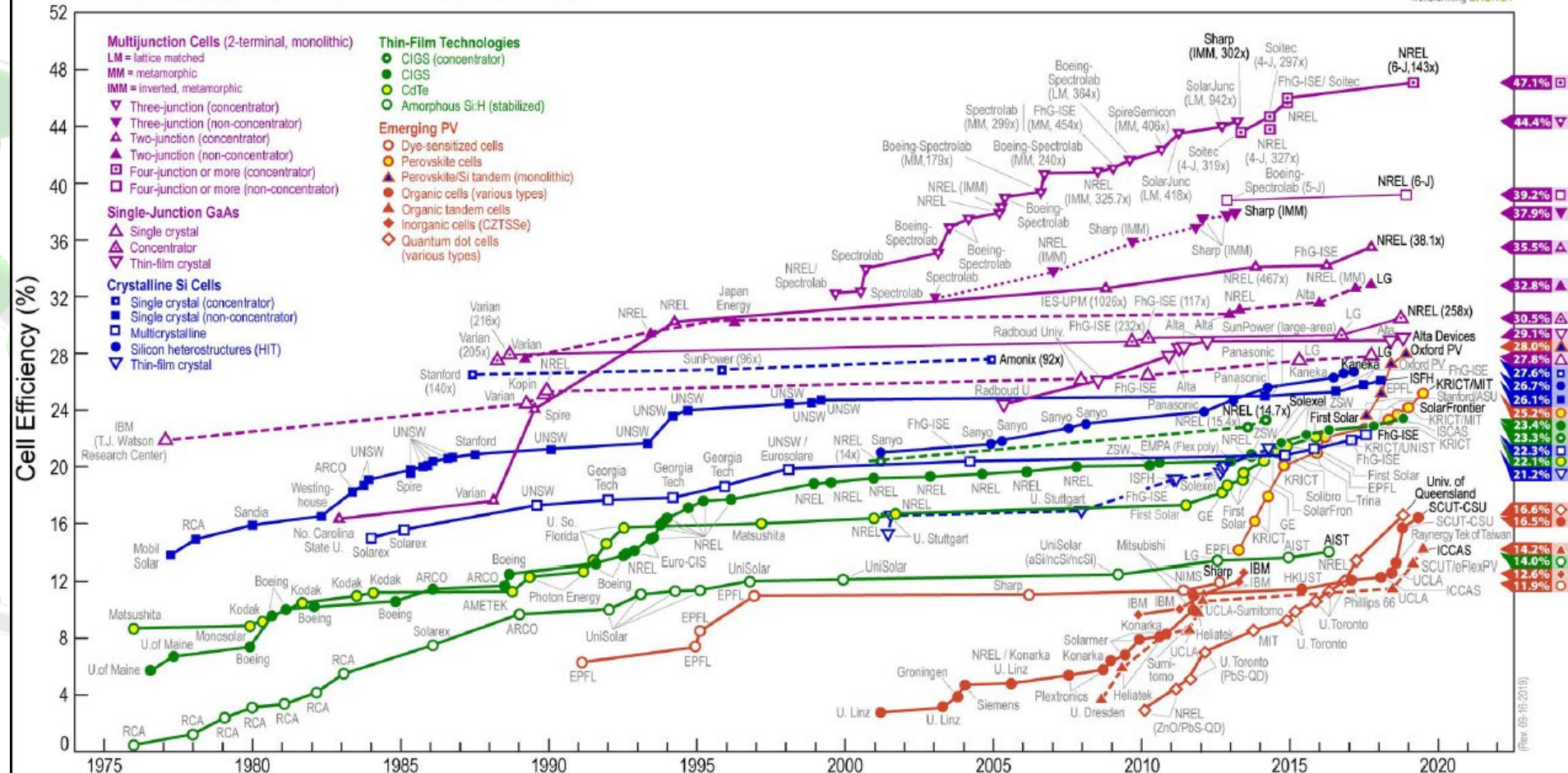
Combination

Industry &  
Social needs



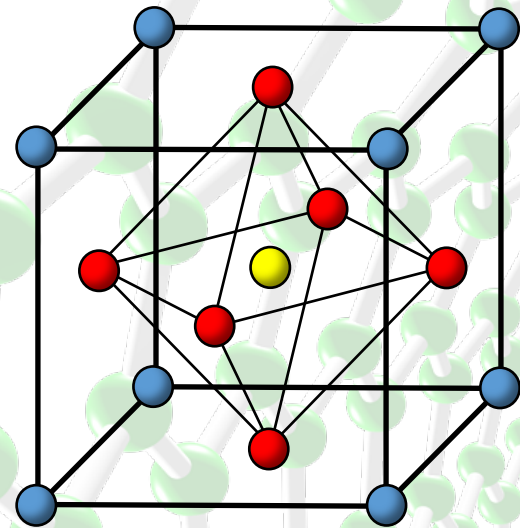
# Solar PV

## Best Research-Cell Efficiencies



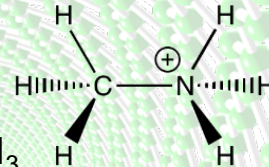
The National Renewable Energy Laboratory (NREL), Best Research-Cell Efficiency Chart, <https://www.nrel.gov/pv/cell-efficiency.html>

# Perovskite Solar Cells

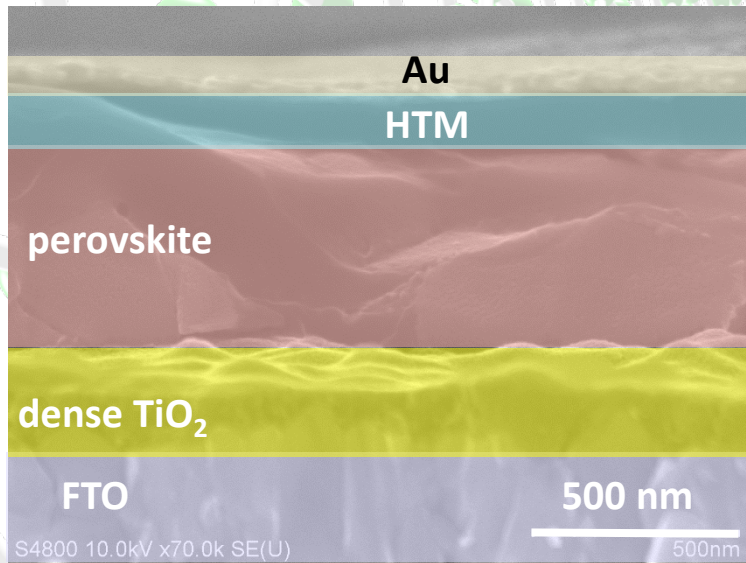
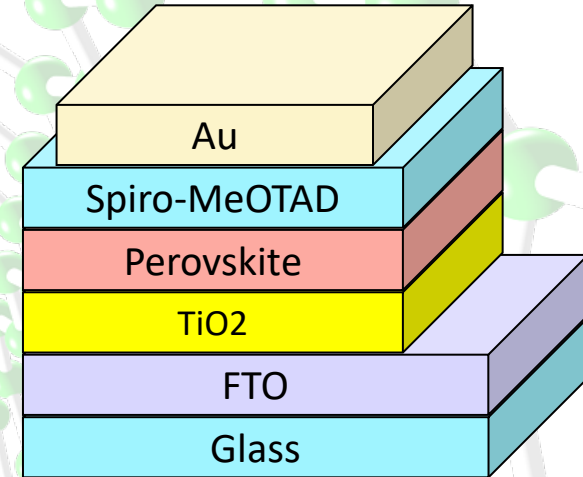


Perovskite:  $AMX_3$

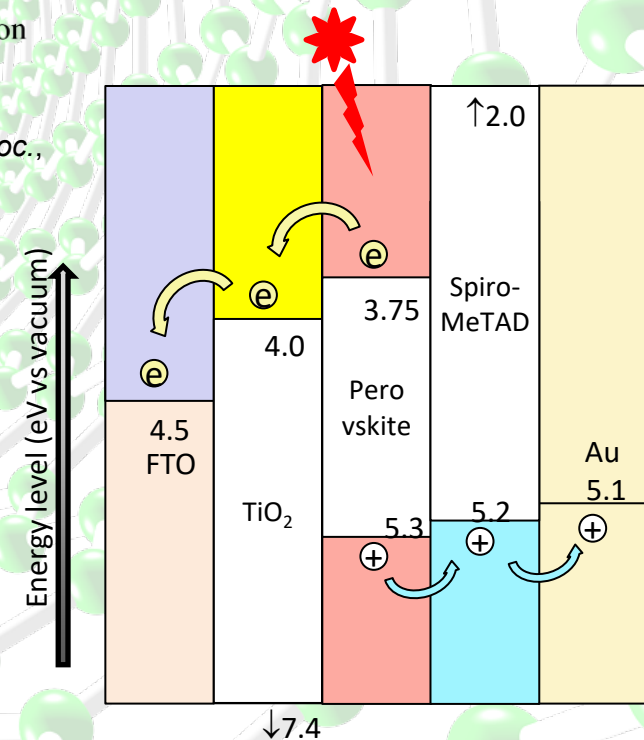
- A = Methylammonium (MA),  $CH_3NH_3^+$   
Formamidinium (FA),  $CH_3(NH_2)_2^+$   
Guanidinium (Gua),  $CH_6N_3^+$
- M =  $Pb^{2+}$ ,  $Sn^{2+}$ ,  $Cs^{2+}$ ,  
 $Rb^{2+}$
- X = I, Cl, Br



methylammonium ion



- Use of Perovskite **PCE 3.8 %**  
A. Kojima, *et al.*, *J. Am. Chem. Soc.*, **2009**
- Solid state solar cell **PCE 10.9 %**  
M. M. Lee, *et al.*, *Science*, **2012**
- High **PCE 20.1 %**  
N. J. Jeon, *et al.*, *Nature*, **2014**
- **PCE record 25.2% 2019**

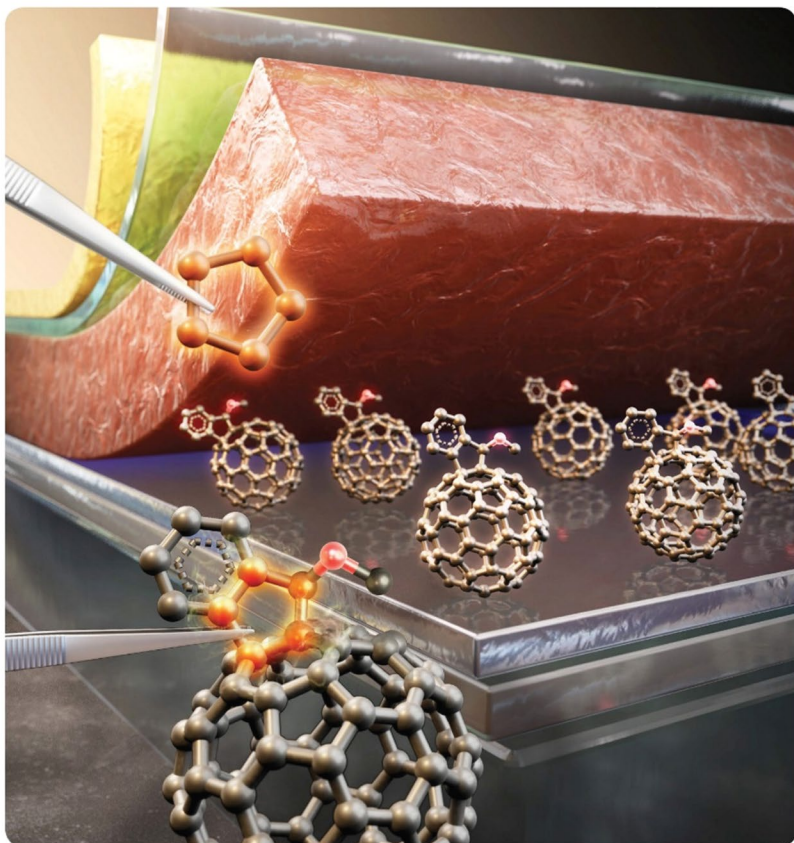




# Passivation Layer

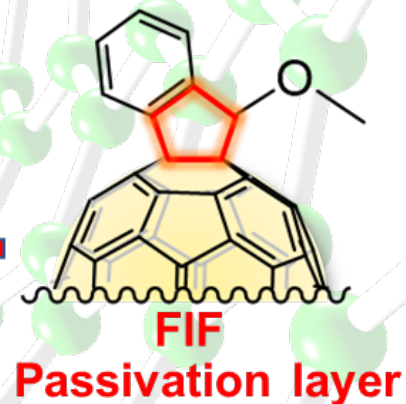
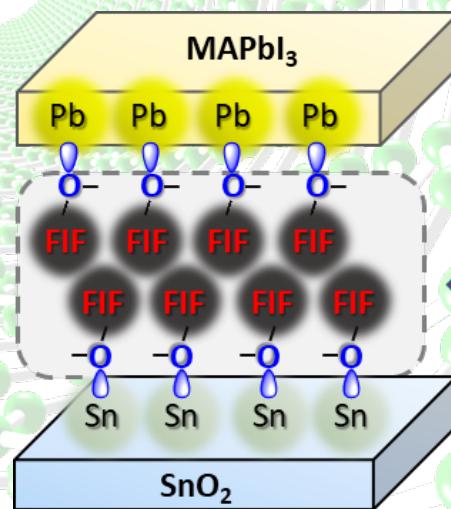
**cm** CHEMISTRY OF MATERIALS

OCTOBER 22, 2019 | VOLUME 31 | NUMBER 20 | pubs.acs.org/cm



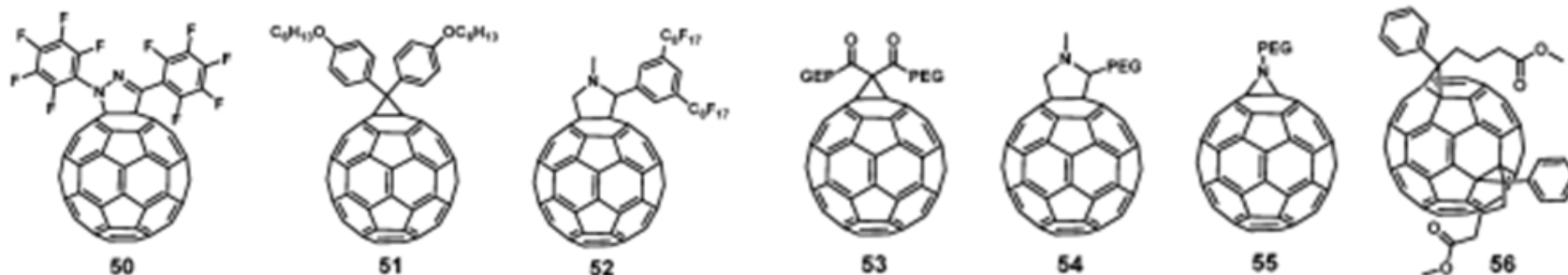
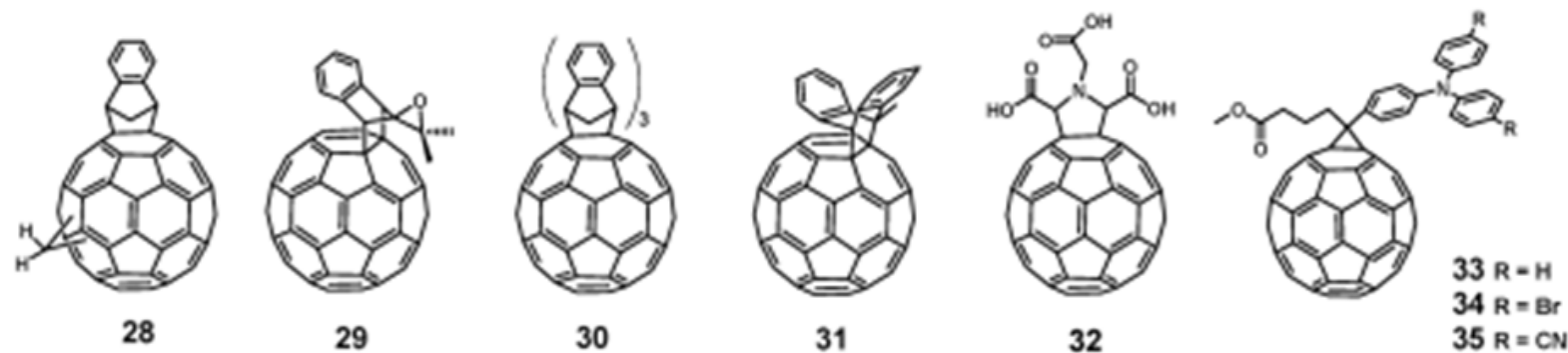
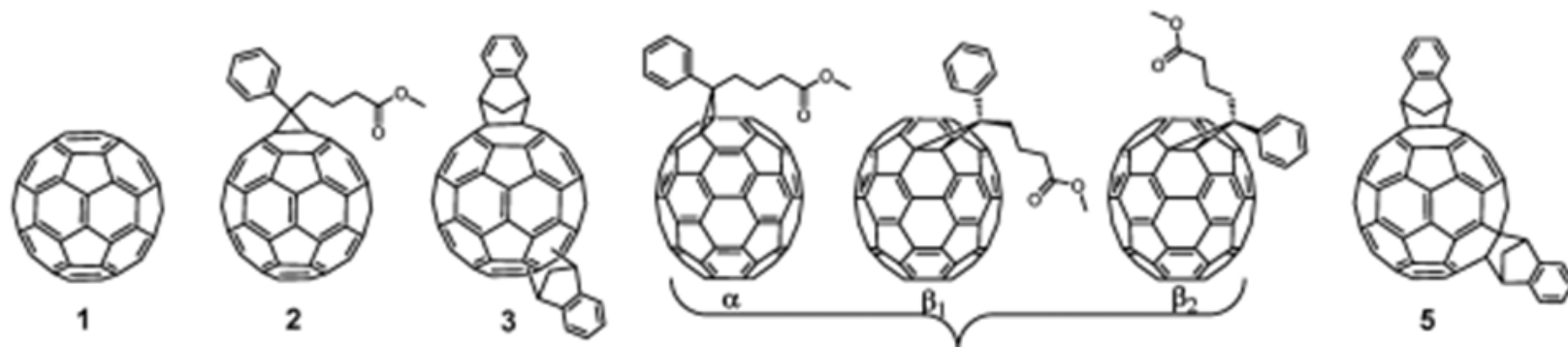
ACS Publications  
Most Trusted. Most Cited. Most Read.

www.acs.org

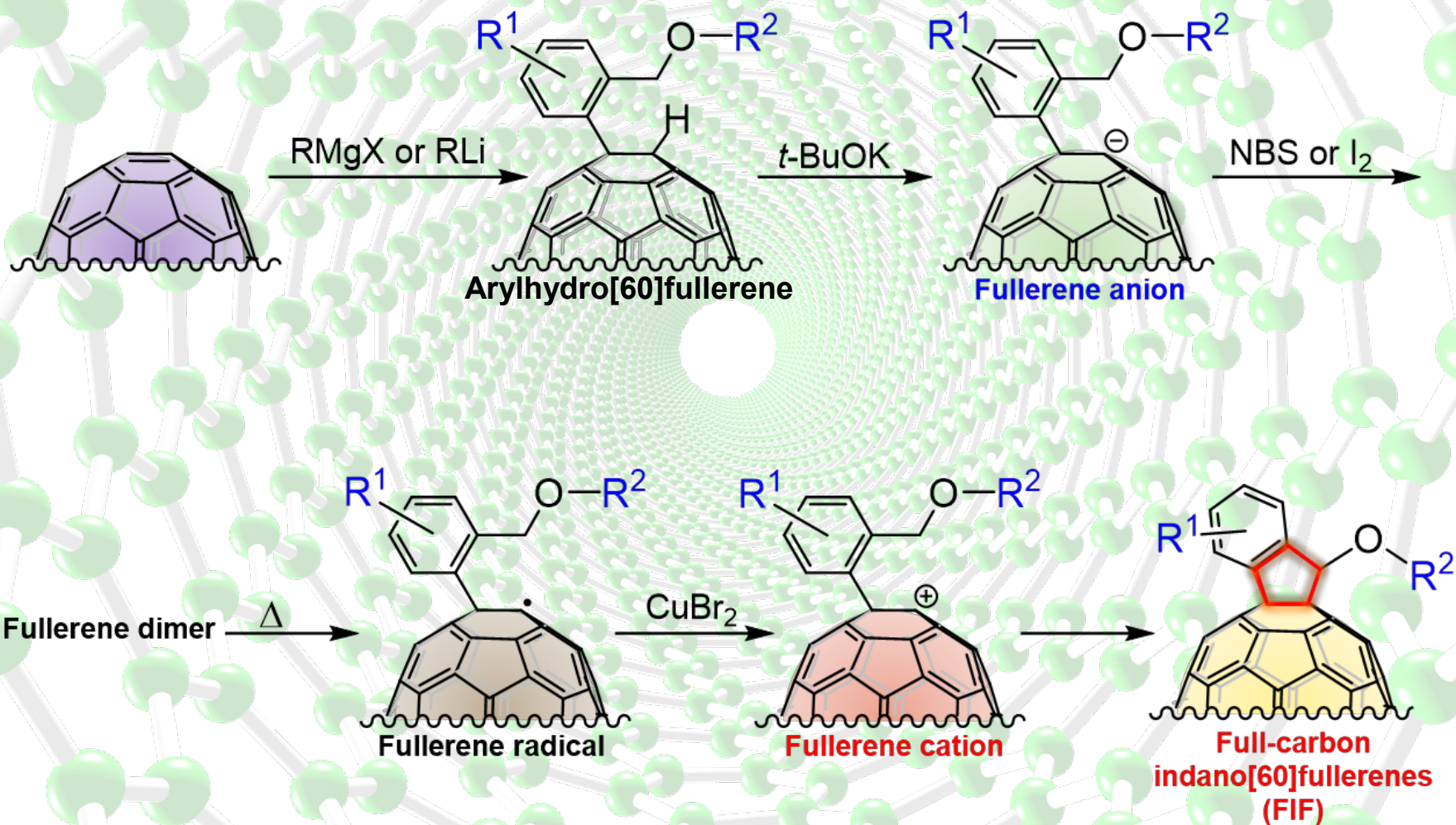


H.-S. Lin, I. Jeon, Y. Chen, X.-Y. Yang, T. Nakagawa, S. Maruyama, S. Manzhos, Y. Matsuo, *Chem. Mater.* **2019**, 31, 8432

# Choice of Molecules



# Molecular Design (=Chemistry)



# Design in Engineering

**Materials**

Choice of materials

**Desired Function**

Needs  
Costs

**Assembly**

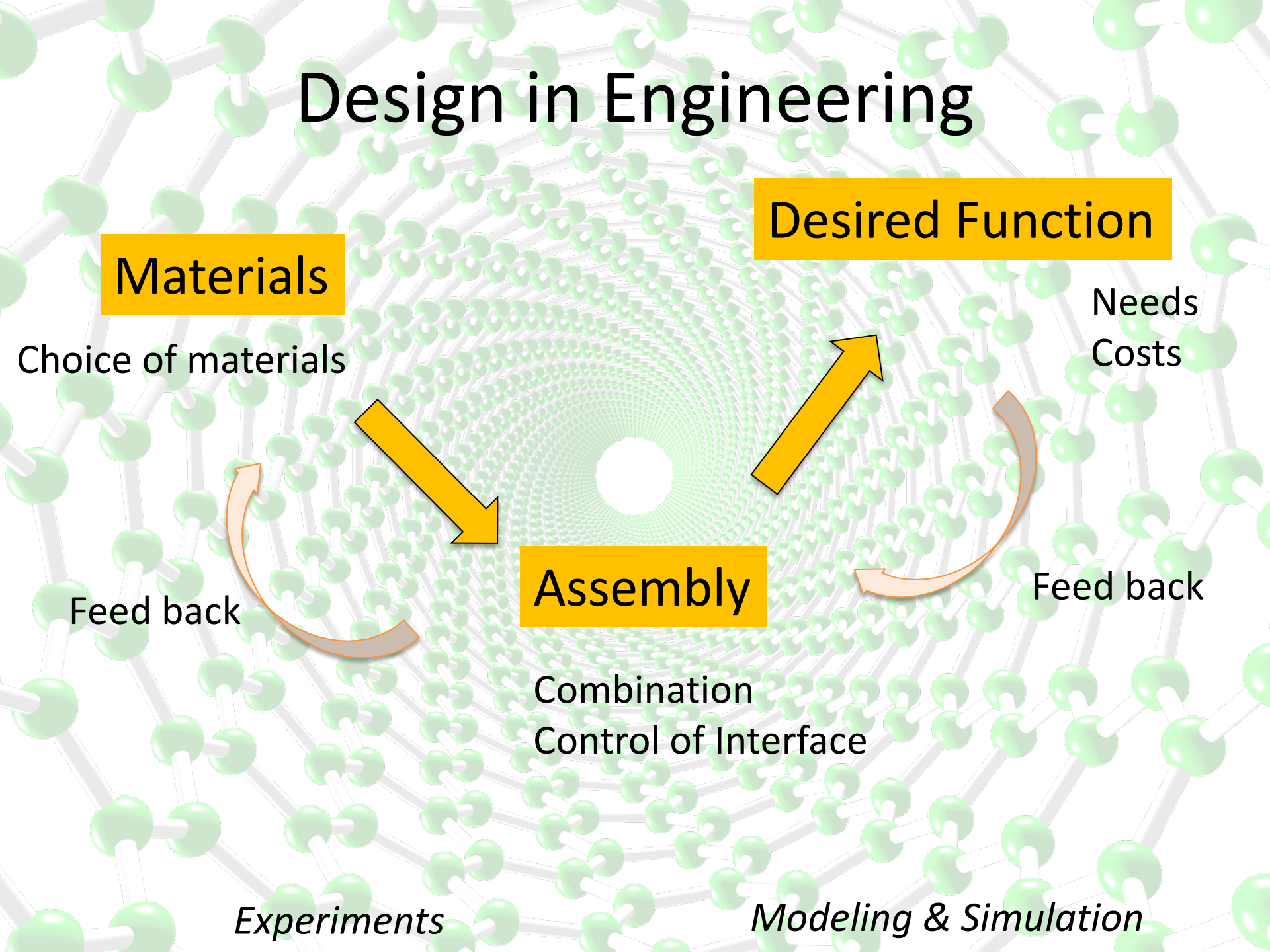
Feed back

Feed back

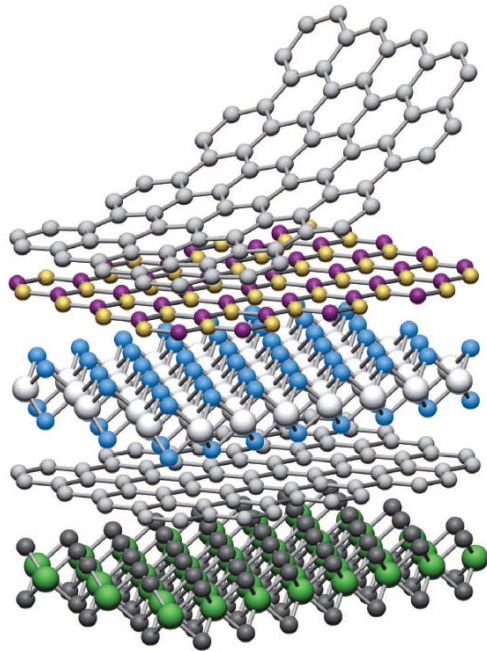
Combination  
Control of Interface

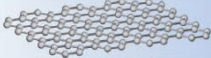

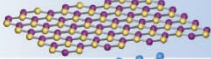



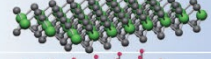

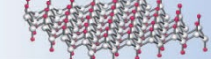

*Experiments*

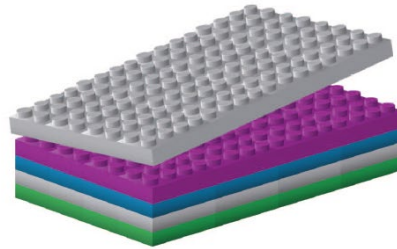
*Modeling & Simulation*



# Design in 1D and 2D materials



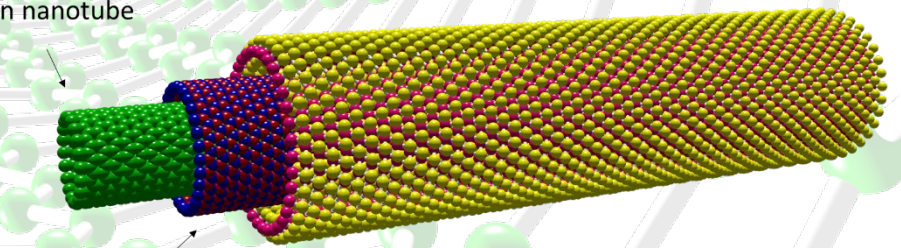
	Graphene	
	hBN	
	MoS <sub>2</sub>	
	WSe <sub>2</sub>	
	Fluorographene	



導電材 (conductor)  
絶縁体 (insulator)  
半導体 (semiconductor)

A. K. Geim & I. V. Grigorieva, *Nature* **499** (2013) 419.

Carbon nanotube



Boron nitride nanotube

MoS<sub>2</sub> nanotube



R. Xiang et al., *Science* **367** (2020) 537.