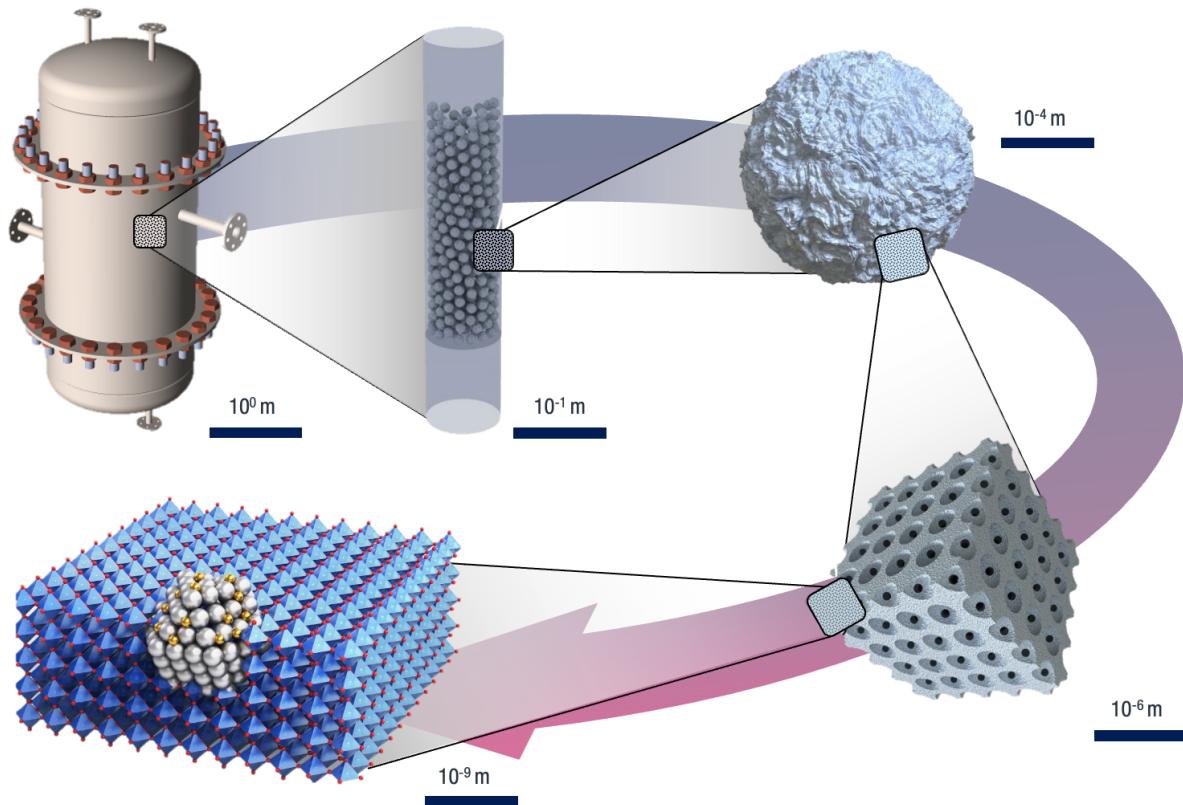


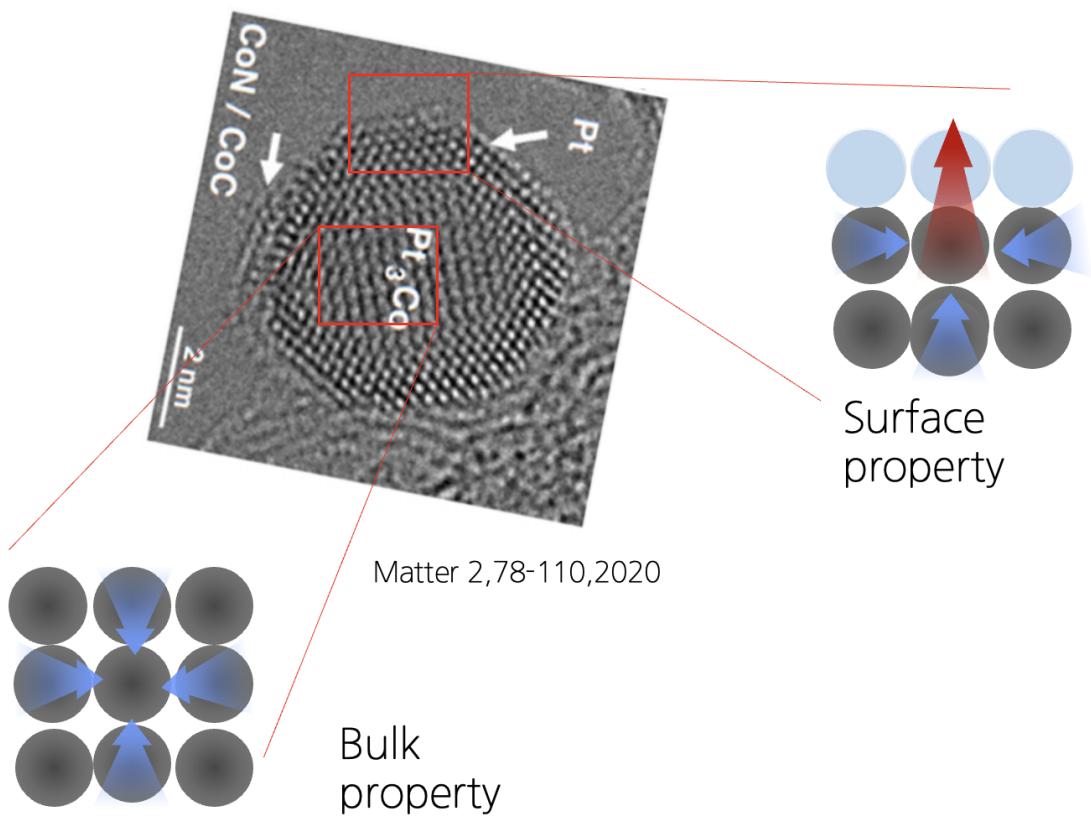


## Hands-on 2. DFT surface

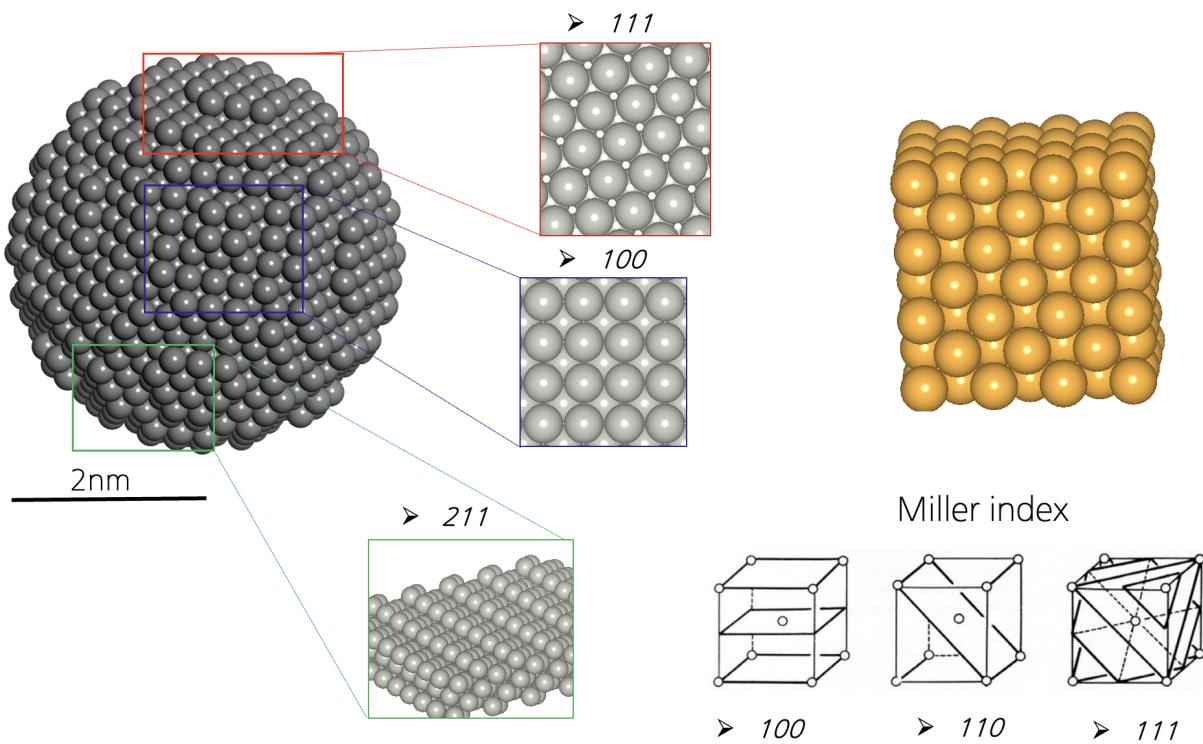
scale of DFT simulations and surface



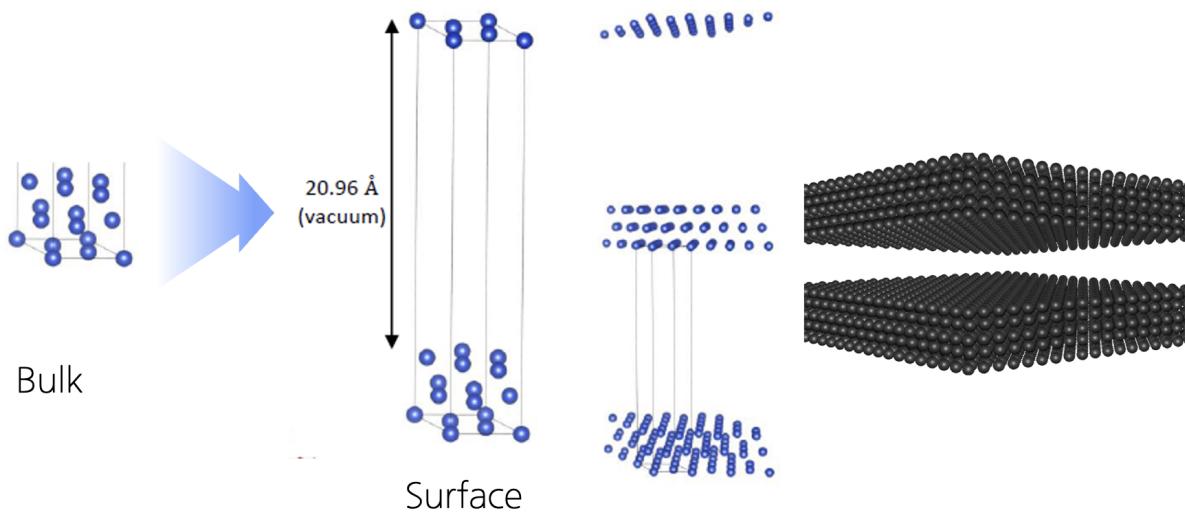
Catalyst surface: undercoordinated surface atoms

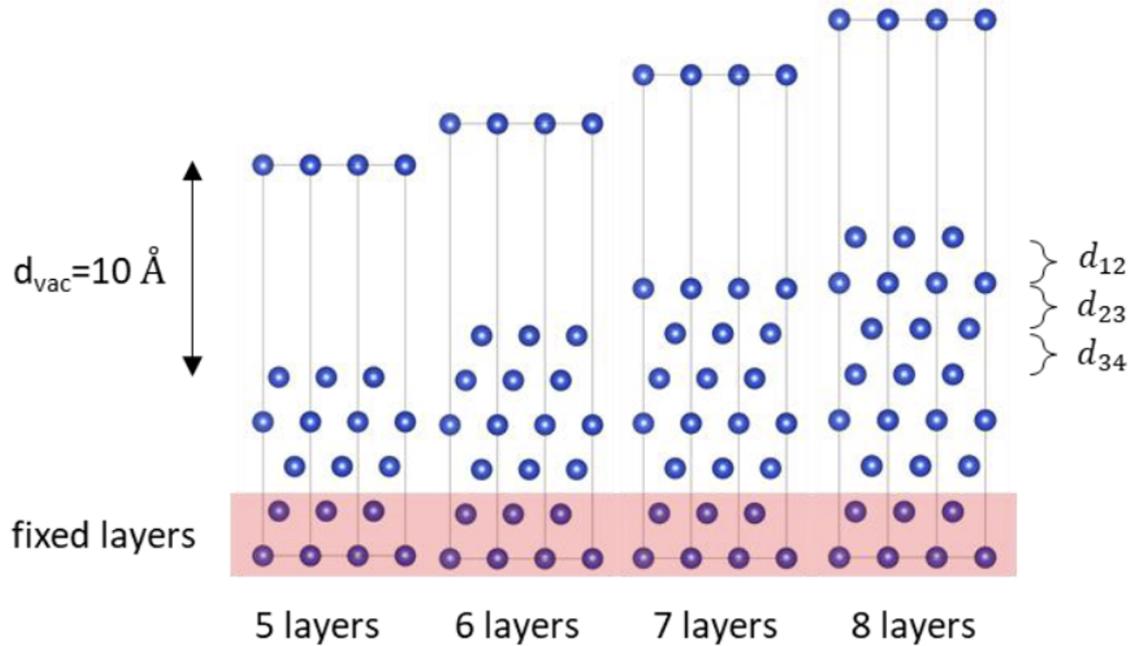


## Catalyst surface facets



## Technical trick to design catalyst surface





Slab model	$\delta d_{12}$ [%]	$\delta d_{23}$ [%]	$\delta d_{34}$ [%]	$\sigma$ [eV/ $\text{\AA}^2$ ]
5 layers	-0.65	0.16	0.02	0.083
6 layers	-0.69	-0.05	0.49	0.085
7 layers	-1.04	0.06	0.30	0.084
8 layers	-0.74	-0.12	0.32	0.085
Expt.	$-0.7 \pm 0.5^a$	-	-	0.114 <sup>b</sup>

<sup>a</sup> Lindgren , S. A°.; Walde'n , L.; Rundgren, J.; Westrin, P. *Phys. Rev. B* **29**, 576 (1984)

<sup>b</sup> de Boer, F. R.; Boom, R.; Mattens, W. C. M.; Miedema, A. R.; Niessen, A. K. *Cohesion in Metals*, North-Holland: Amsterdam, 1988.

$$\sigma = \frac{1}{A} [E_{\text{slab}} - nE_{\text{bulk}}]$$

**TABLE 4.2** Surface Energies Calculated for Cu(100) and Cu(111) from DFT as Function of Slab Thickness, in eV/ $\text{\AA}^2$  (J/m<sup>2</sup>)<sup>a</sup>

Slab Model	$\sigma$ , Cu(100)	$\sigma$ , Cu(111)
5 layers	0.094 (1.50)	0.087 (1.40)
6 layers	0.097 (1.55)	0.089 (1.43)
7 layers	0.098 (1.57)	0.089 (1.43)
8 layers	0.096 (1.53)	0.091 (1.46)
Expt.		0.114 (1.83) <sup>b</sup>

# Assignment

Please **select one metal element (from the red box)** and complete the following tasks:

1. **Run a catalyst surface simulation** for the chosen metal. Calculate the surface energy using a total of 6 layers, with the bottom 3 layers fixed and the top 3 layers relaxed. It is recommended to use k-points of  $4\times4\times1$  and a plane wave cutoff of 400 eV. If the simulation is too slow, you may reduce the k-points to  $1\times1\times1$  and PW cutoff 300 eV.
2. **Vary the number of layers** and observe how the surface energy changes.
3. **Compare the surface energies** of the (100), (110), and (111) facets.

Please submit your results along with a **concise explanation of your findings, limited to one page. (format: studentnumber\_name.doc (.pdf or whatever), ex)12345\_seokhyunchoung.doc)**

	27						
		Co	Ni	Cu			
2	Cobalt	Nickel	Copper				
	3d7 4s2	3d8 4s2	3d10 4s1				
	58.93	58.69	63.55				
	45	46	47				
	Rh	Pd	Ag				
1	Rhodium	Palladium	Silver				
	4d8 5s1	4d10	4d10 5s1				
	102.9	106.4	107.9				
	77	78	79				
	Ir	Pt	Au				
n	Iridium	Platinum	Gold				
6s2	4f14 5d7 6s2	4f14 5d9 6s1	4f14 5d10 6s1				
	192.2	195.1	197				