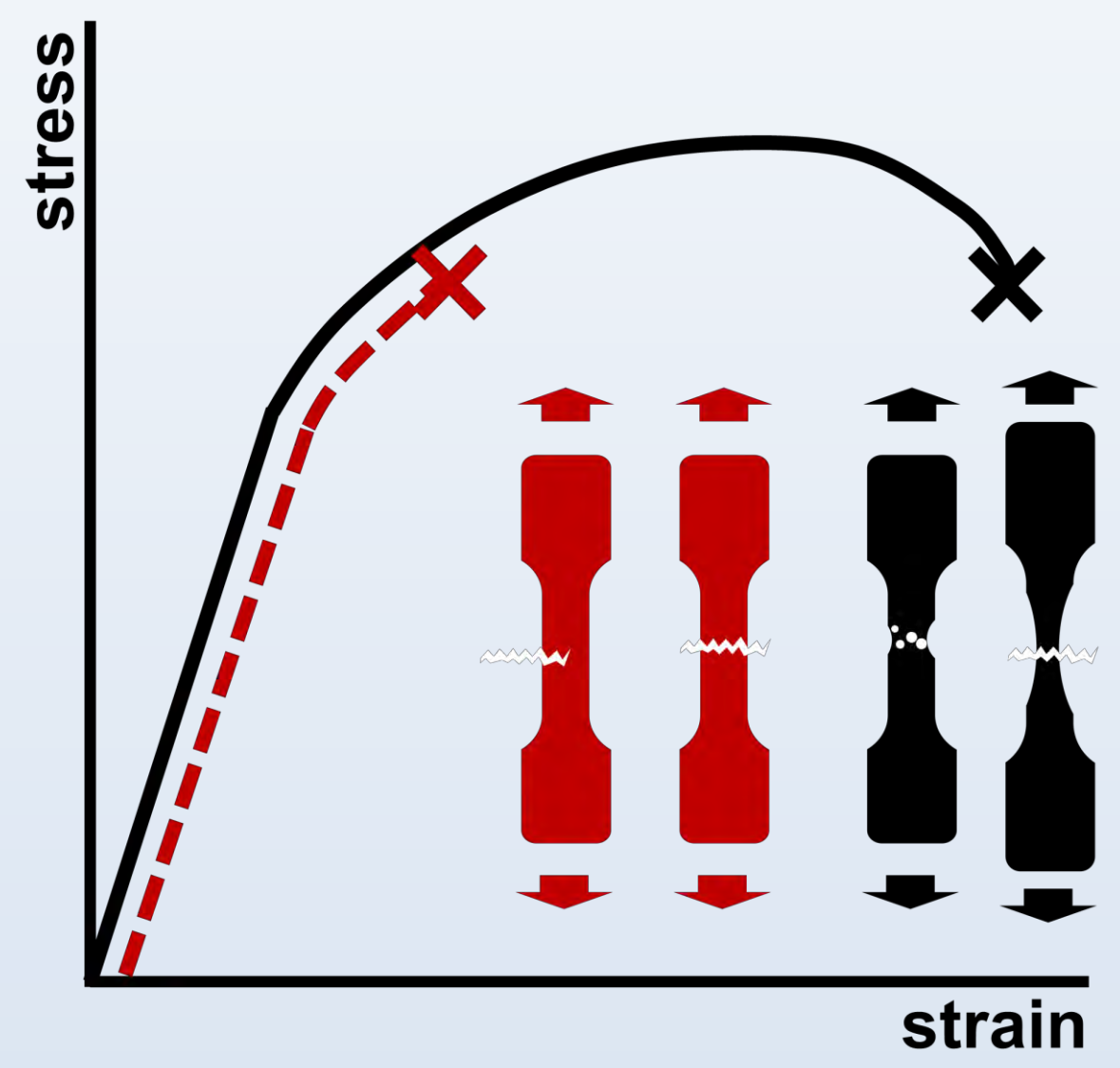# Effect of alloying element on hydrogen concentration
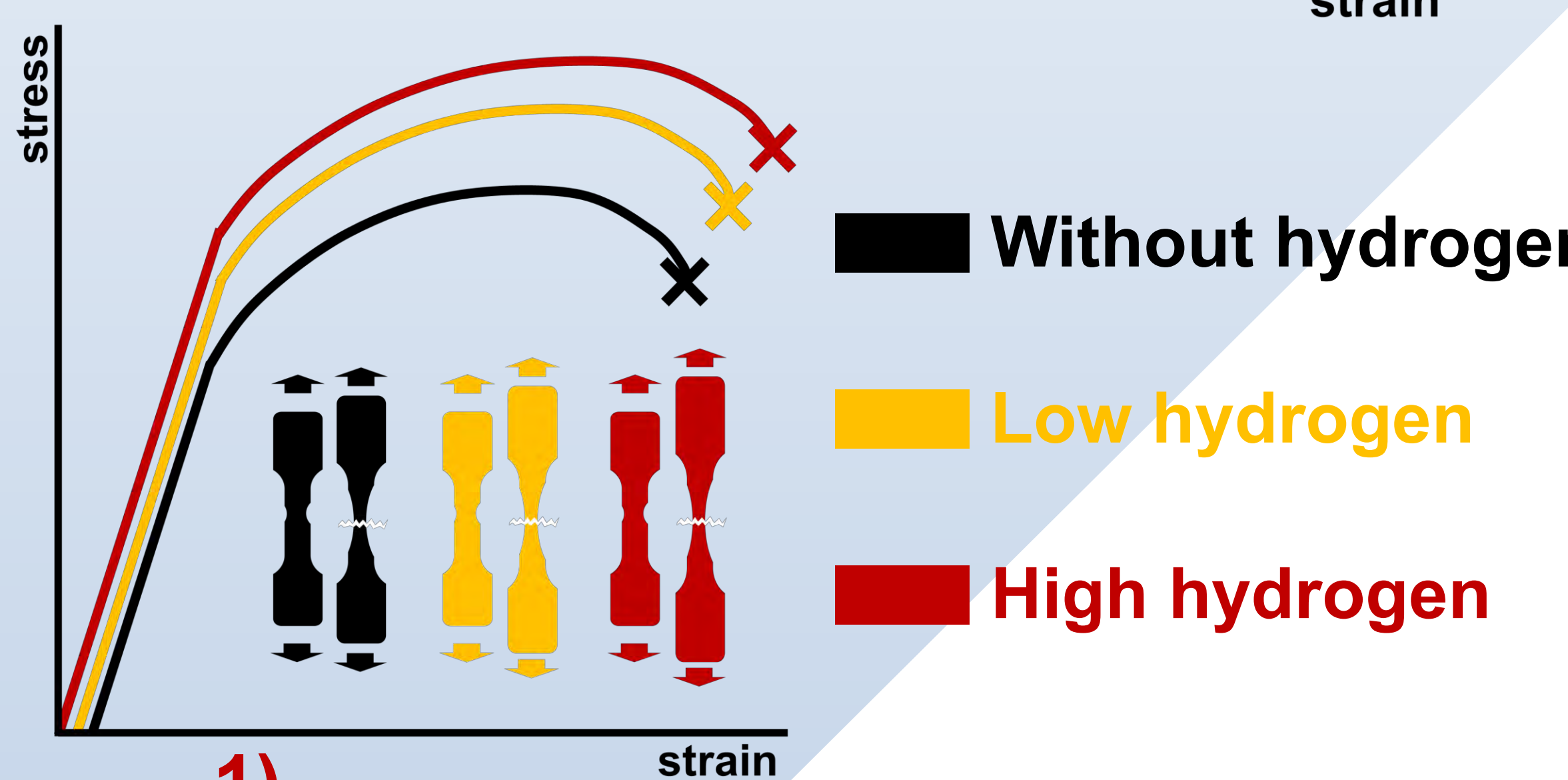
Fe-Cr-Ni alloy with Hydrogen

Prediction of hydrogen concentration by computational method
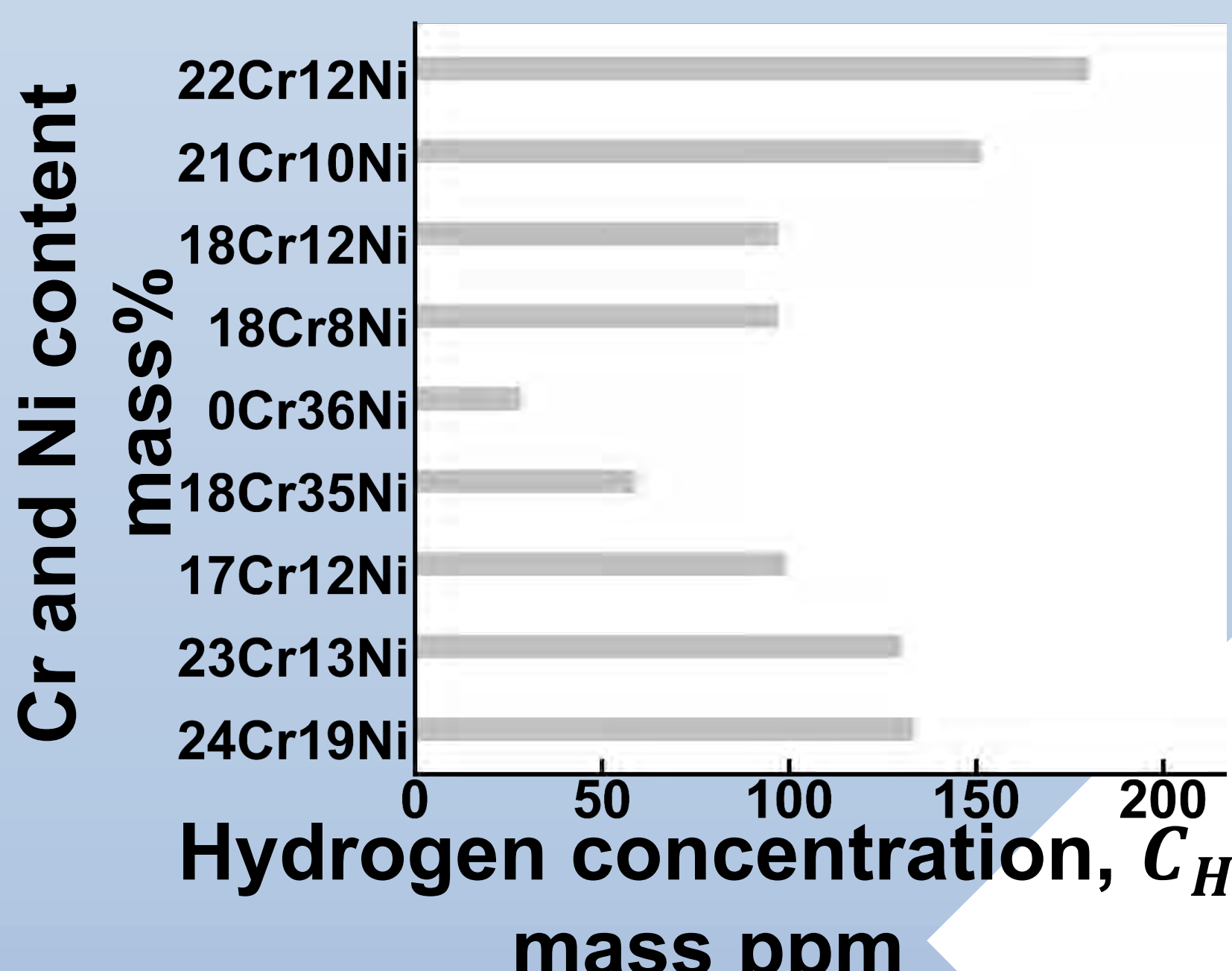Moriyama Junichiro D1 Mechanical engineering department

In general …
Hydrogen **reduces** strength and ductility. (Hydrogen embrittlement)

stress / strain

However …
Hydrogen **enhances** strength and ductility in some Fe-Cr-Ni alloy[1].
**This effect more pronounced as hydrogen concentration increases[1].**

stress / strain

Without hydrogen
Low hydrogen
High hydrogen

Hydrogen concentration…
depends on the chemical composition of **Cr and Ni[2),3)]**.

Cr and Ni content mass%:
22Cr12Ni, 21Cr10Ni, 18Cr12Ni, 18Cr8Ni, 0Cr36Ni, 18Cr35Ni, 17Cr12Ni, 23Cr13Ni, 24Cr19Ni

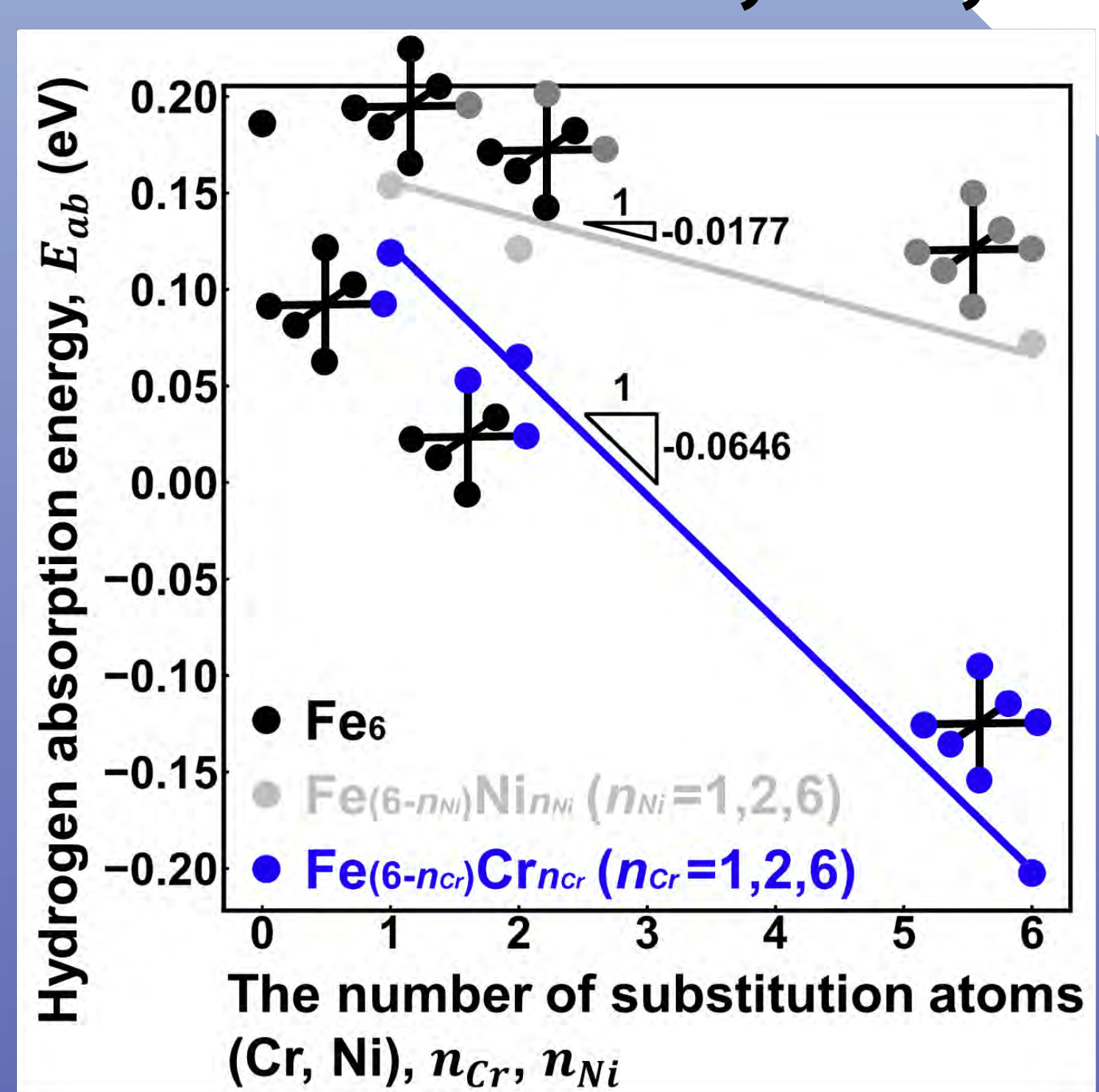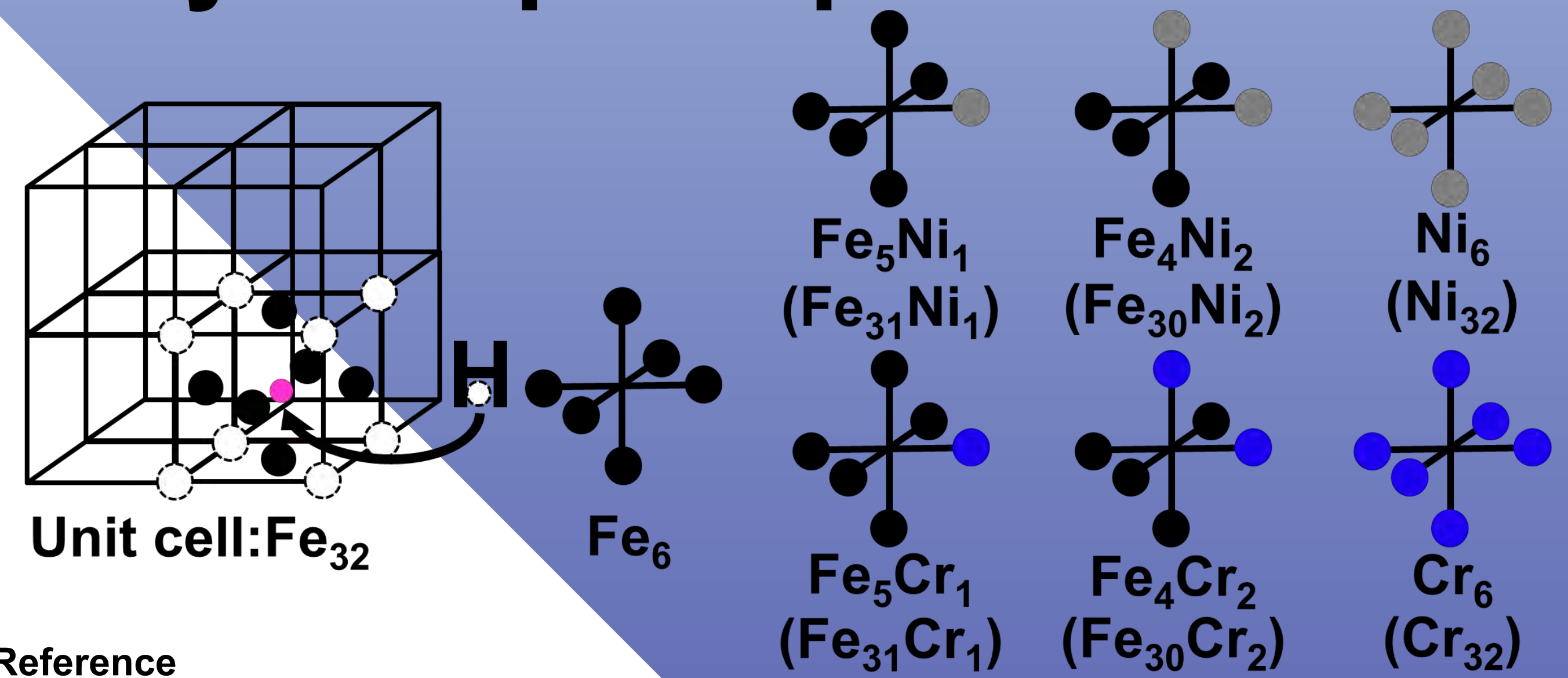Hydrogen concentration, C_H mass ppm (0, 50, 100, 150, 200)

Purpose
Predict hydrogen concentration due to evaluate hydrogen absorption energy by using first-principles calculation.

Hydrogen absorption energy?
The energy to insert hydrogen atom to the alloy.

H
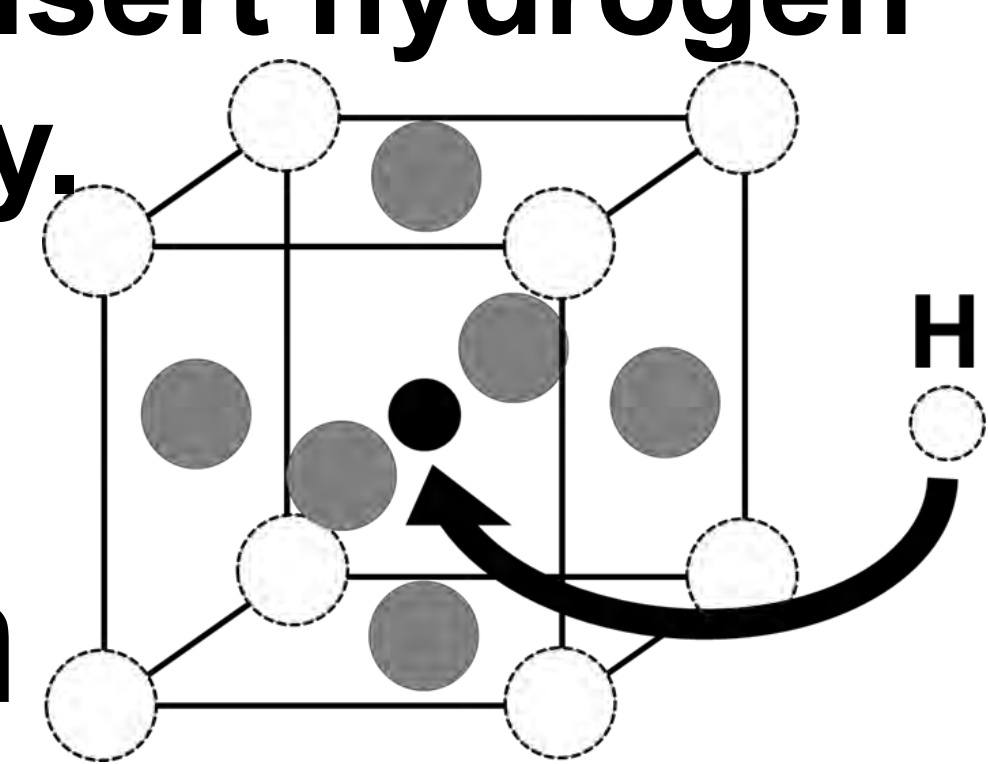
Prediction method

1. Calculate hydrogen absorption energy, E_{ab} in octahedral site which was consisted of Fe, Cr, Ni atom by first-principles calculation

Unit cell: Fe$_{32}$

H

Fe$_6$

Fe$_5$Ni$_1$ (Fe$_{31}$Ni$_1$) Fe$_4$Ni$_2$ (Fe$_{30}$Ni$_2$) Ni$_6$ (Ni$_{32}$)

Fe$_5$Cr$_1$ (Fe$_{31}$Cr$_1$) Fe$_4$Cr$_2$ (Fe$_{30}$Cr$_2$) Cr$_6$ (Cr$_{32}$)

Hydrogen absorption energy, E_{ab} (eV)

1 : -0.0177
1 : -0.0646

Fe$_6$
Fe$_{(6-n_{Ni})}$Ni$_{n_{Ni}}$ (n_{Ni}=1,2,6)
Fe$_{(6-n_{Cr})}$Cr$_{n_{Cr}}$ (n_{Cr}=1,2,6)

The number of substitution atoms (Cr, Ni), n_{Cr}, n_{Ni}

$$E_{ab} = 0.186 - 0.0646 n_{Cr} - 0.0177 n_{Ni}$$

Cr and Ni **decrease** hydrogen absorption energy (increase hydrogen concentration)

Reference
1) Y. Ogawa et al., Acta Mater. 199 (2020) 181–192.
2) J. Yamabe et al., Int. J. Hydrogen Energy. 42 (2017) 13289–13299
3) H.Nishida et al., Mater. Sci. Eng. A. 836 (2022) 142681.

2. Calculate hydrogen concentration, C_H from hydrogen absorption energy

Atomic ratio of Cr and Ni of 24Cr-19Ni
Cr : 0.255   Ni : 0.179

$$E_{ab} = 0.186 - 0.0646 n_{Cr} - 0.0177 n_{Ni}$$

$$\theta_L = \frac{1}{1 + exp\left(\frac{E_{ab} - \mu^*}{k_B T}\right)}$$
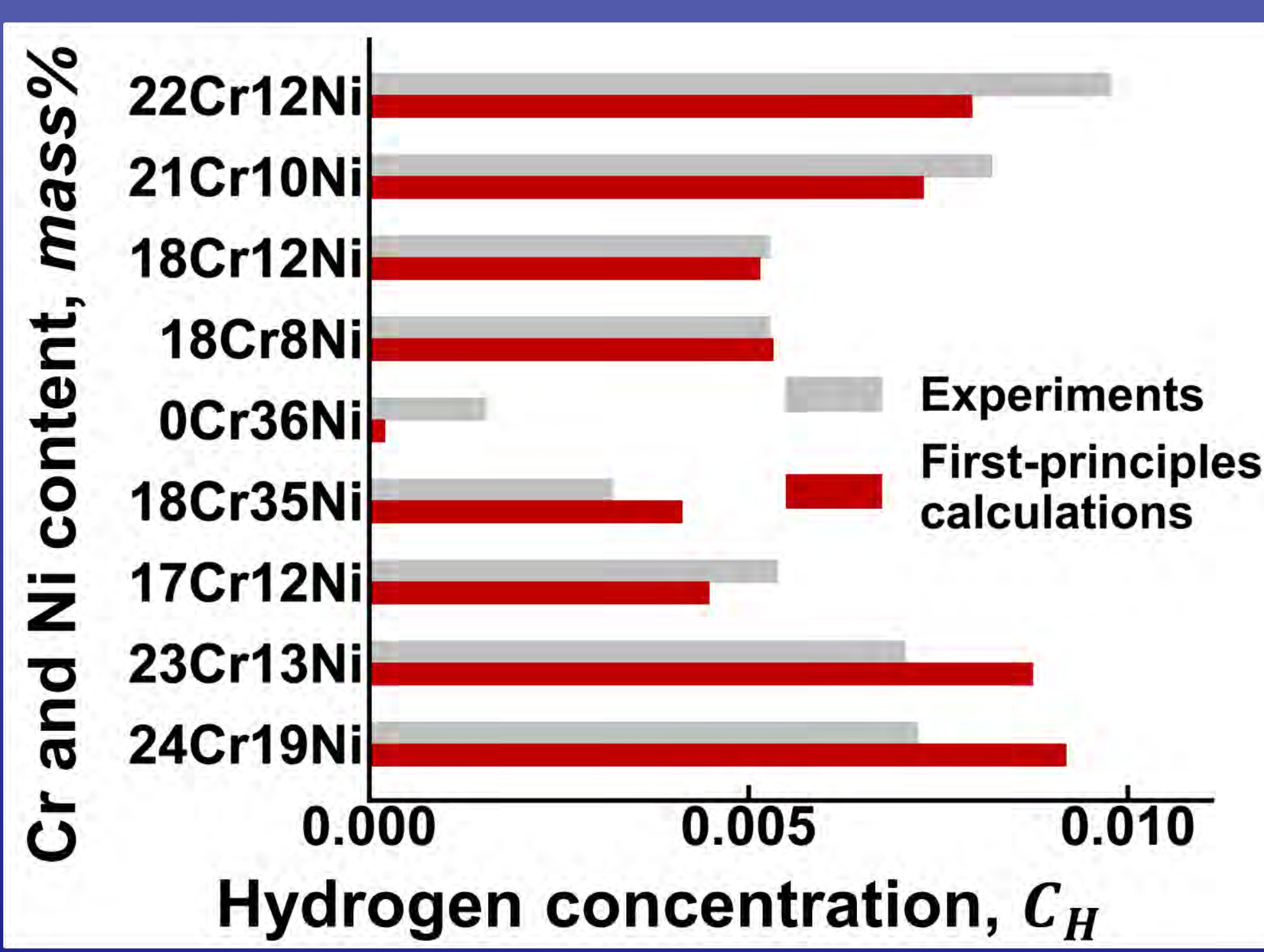
Average $\theta_L = C_H$

Procedure
1. Randomly generated 100000 patterns of 6 combinations of Fe, Cr, Ni (octahedral site) with atomic ratio of alloys as probability.
2. Calculate hydrogen absorption energy for each octahedral site.
3. From hydrogen absorption energy E_{ab}, calculate hydrogen occupancy for each octahedral site.
4. Average hydrogen occupancy.

Cr and Ni content, mass%:
22Cr12Ni, 21Cr10Ni, 18Cr12Ni, 18Cr8Ni, 0Cr36Ni, 18Cr35Ni, 17Cr12Ni, 23Cr13Ni, 24Cr19Ni

Experiments
First-principles calculations

Hydrogen concentration, C_H (0.000, 0.005, 0.010)

The Calculated hydrogen concentration corresponds to the experimental result.