

# First principles calculations of stacking fault energy of P doped Si crystal

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Obrigado, moderador.

Boa tarde, senhores e senhoras,

Sou Prof. Shigeto Robert Nishitani do Universidade Kwansei Gakuin, que localiza no oeste do Japão.

O Brasil me lembrar o famoso ganhador(winner) do Prêmio Nobel Richard Feynman , seu livro popular "O senhor está brincando, Sr. Feynman!"

Isso é minha origem de fazer alguma coisa em abordagem teórica para a ciência de materiais.

Depois de vinte anos, estou ainda batalhando com física difícil,

mas graça do Calphad Meeting e seu organizador principal, professor Andre Costa de Silva,

estou um poquinho(little) familiar com o português,

# Si-wafers(300mm $\Phi$ )

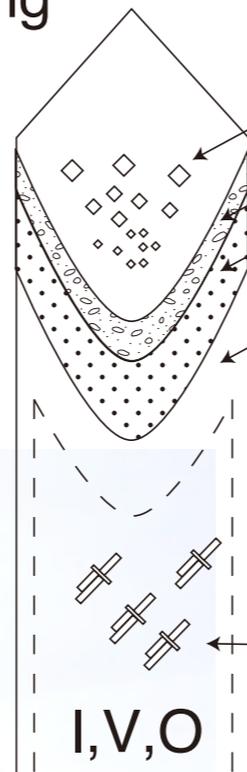
Shin-Etsu+SUMCO (share 50%)

Yakawa(Shinetsu) (share 22%)

Shin-Etsu



Cooling



Vacancy type

Interstitial type

Interstitial type

Vacancy type

dislocation loops

Melt

Defects density

Growth rate

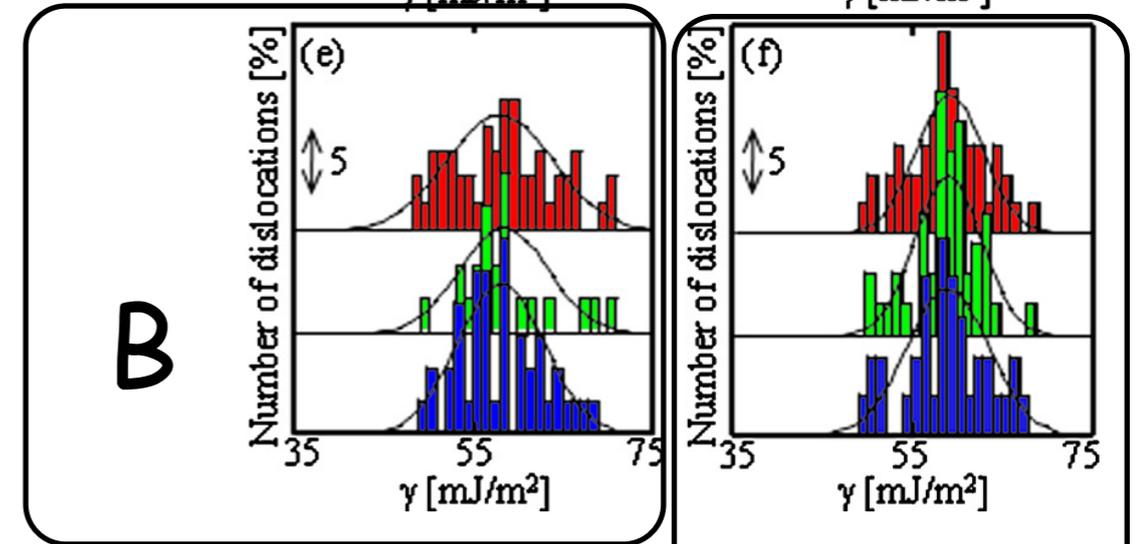
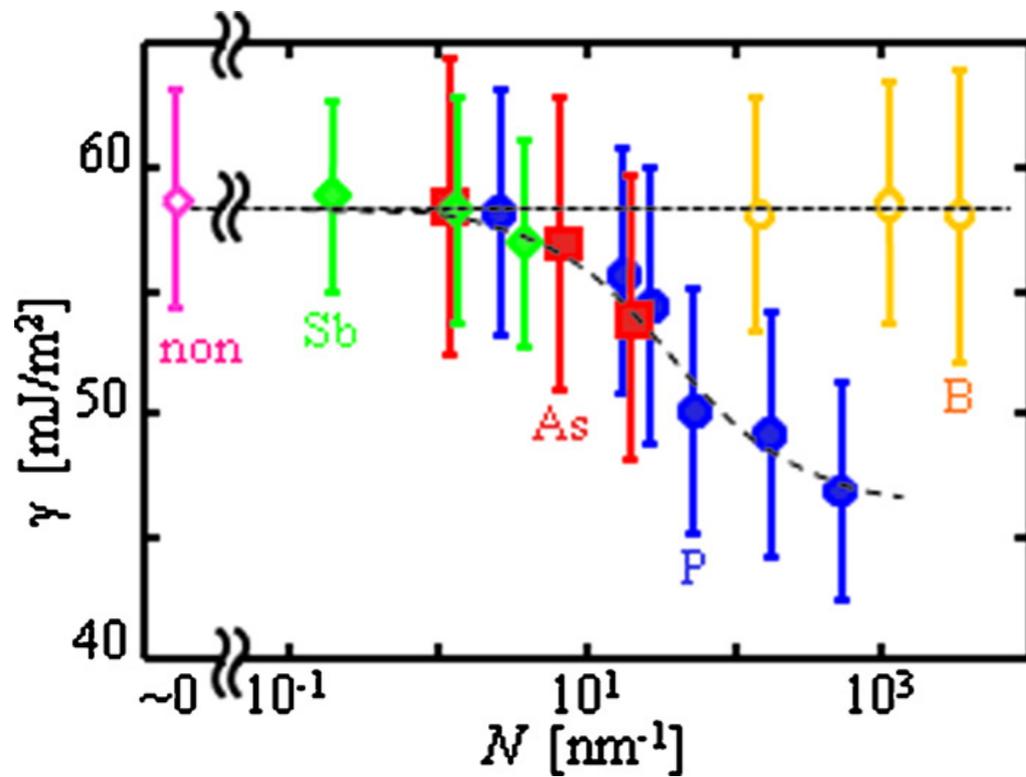
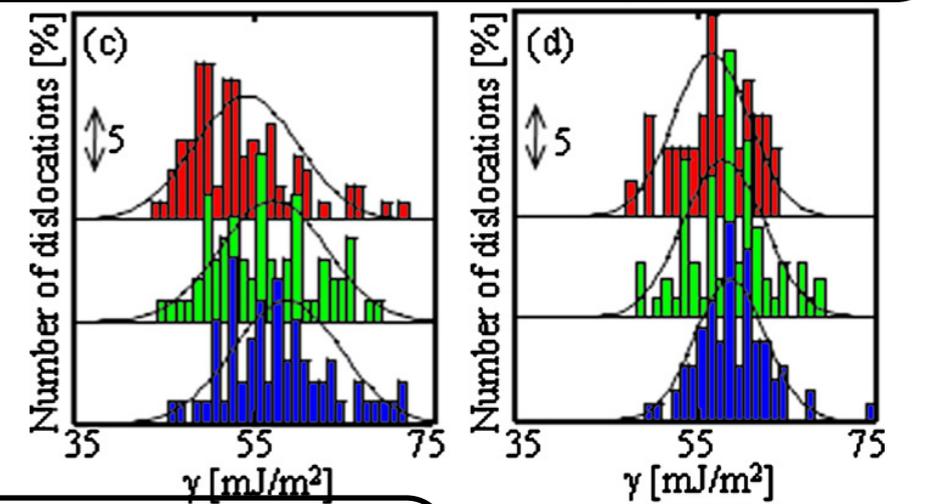
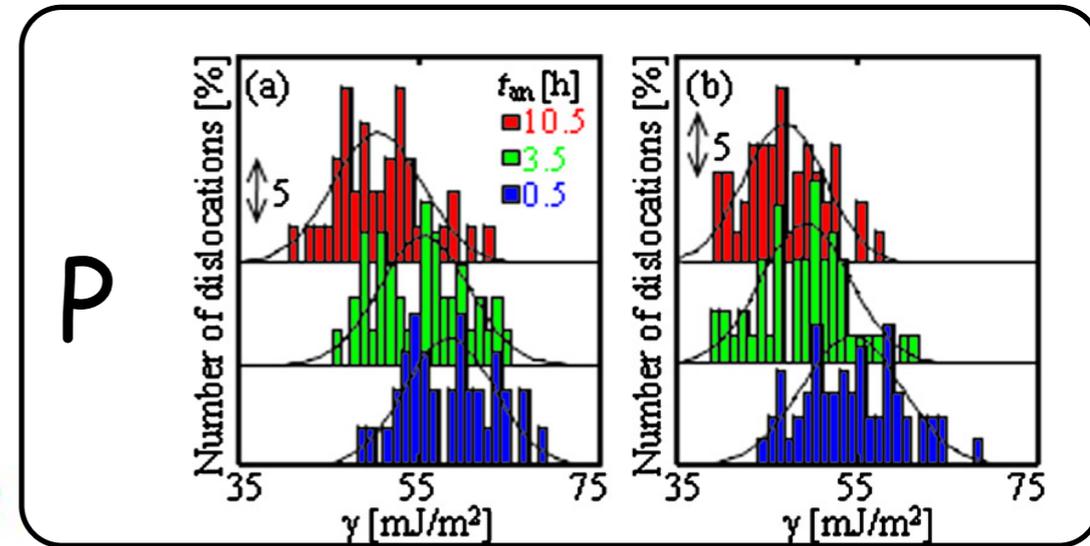
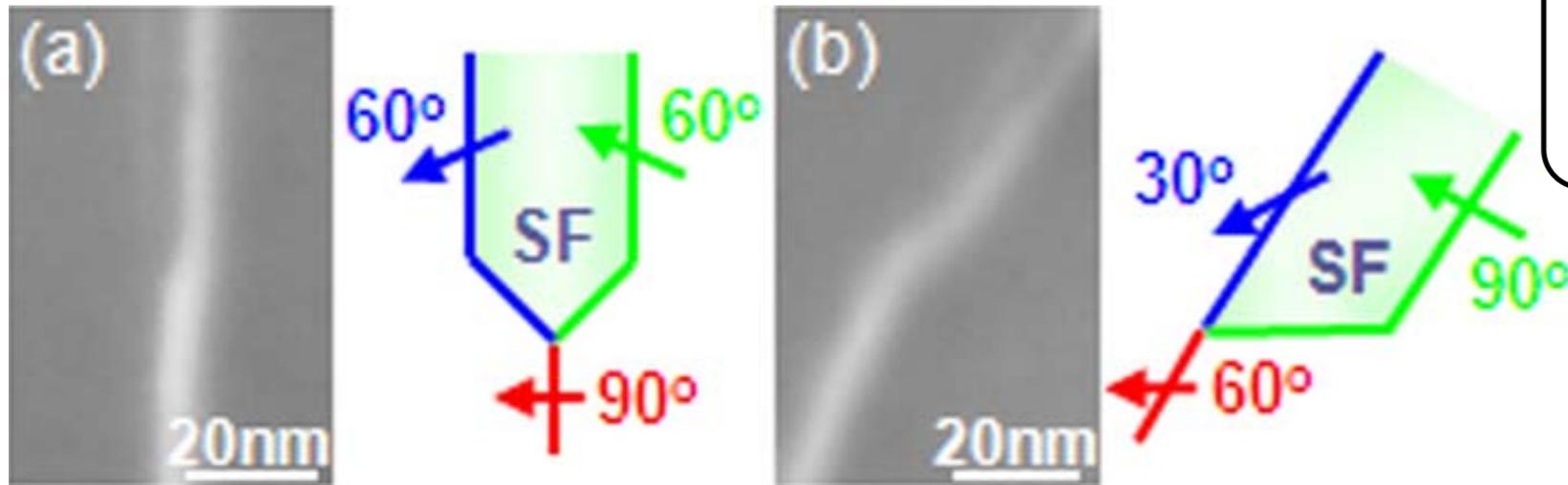
dislocation loops

N<sub>i</sub> N<sub>v</sub>

voids

OSF ring

# Ohno's results



non-doped

# For Fe

Ishida & Nishizawa,  
Nippon Kinzoku  
Gakkaishi,  
36(1972), 1238

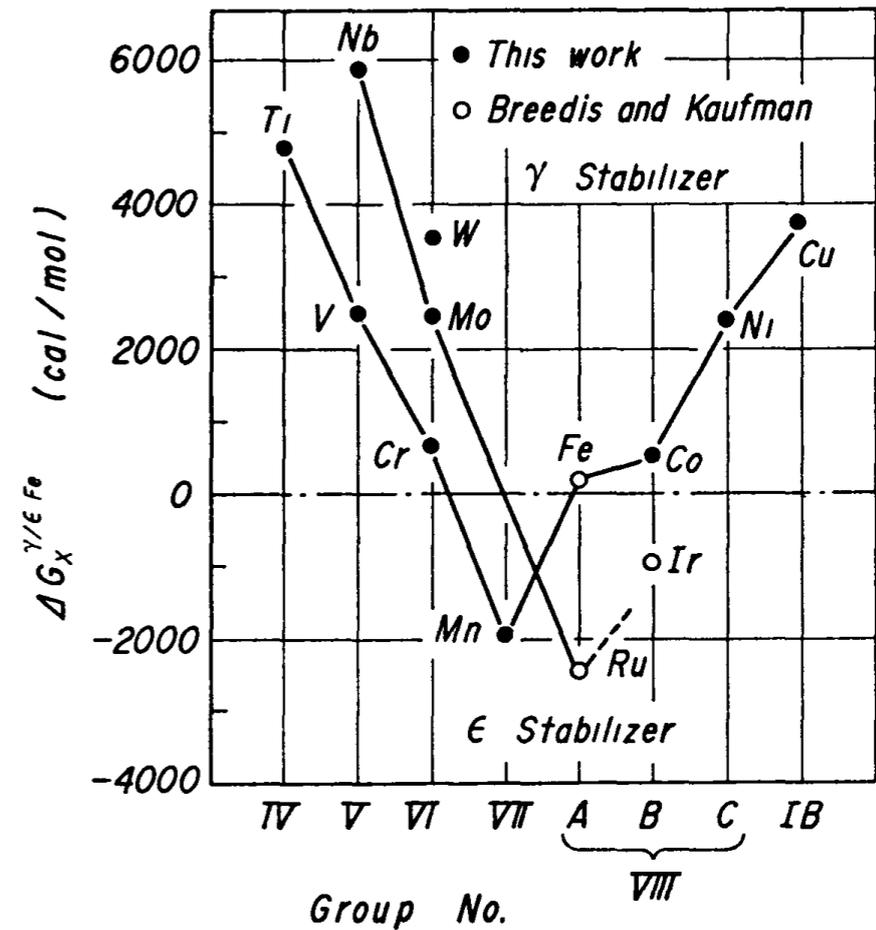
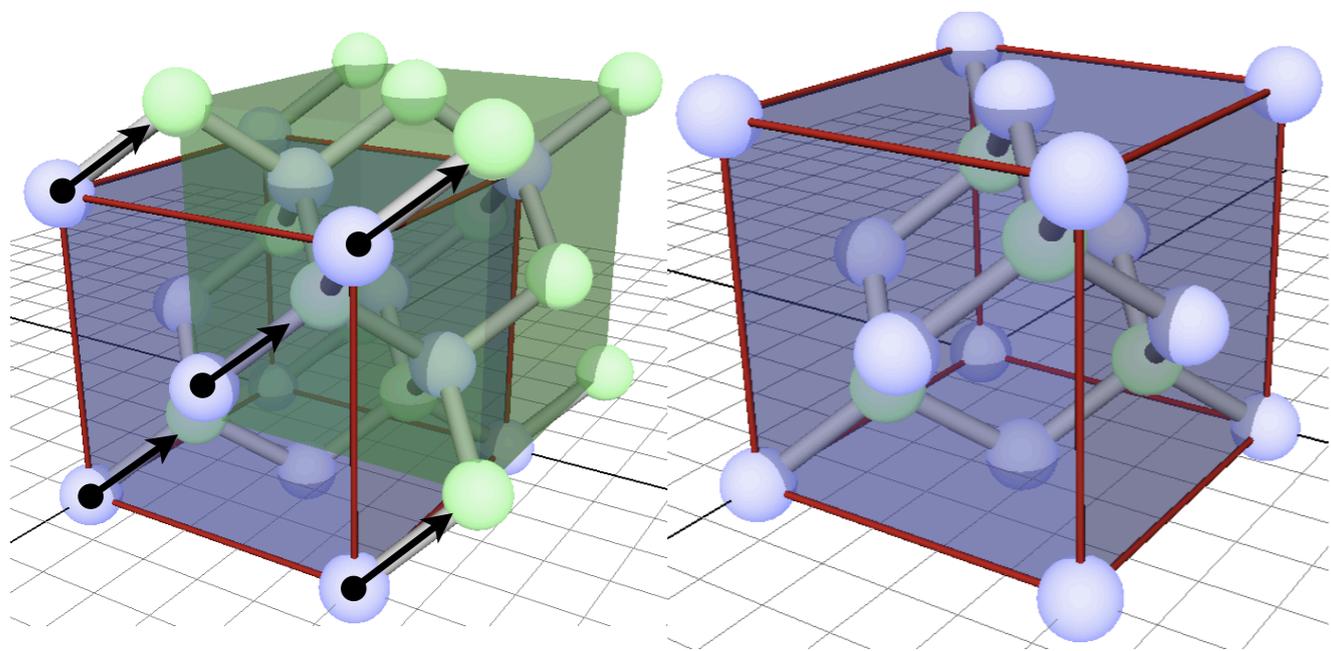


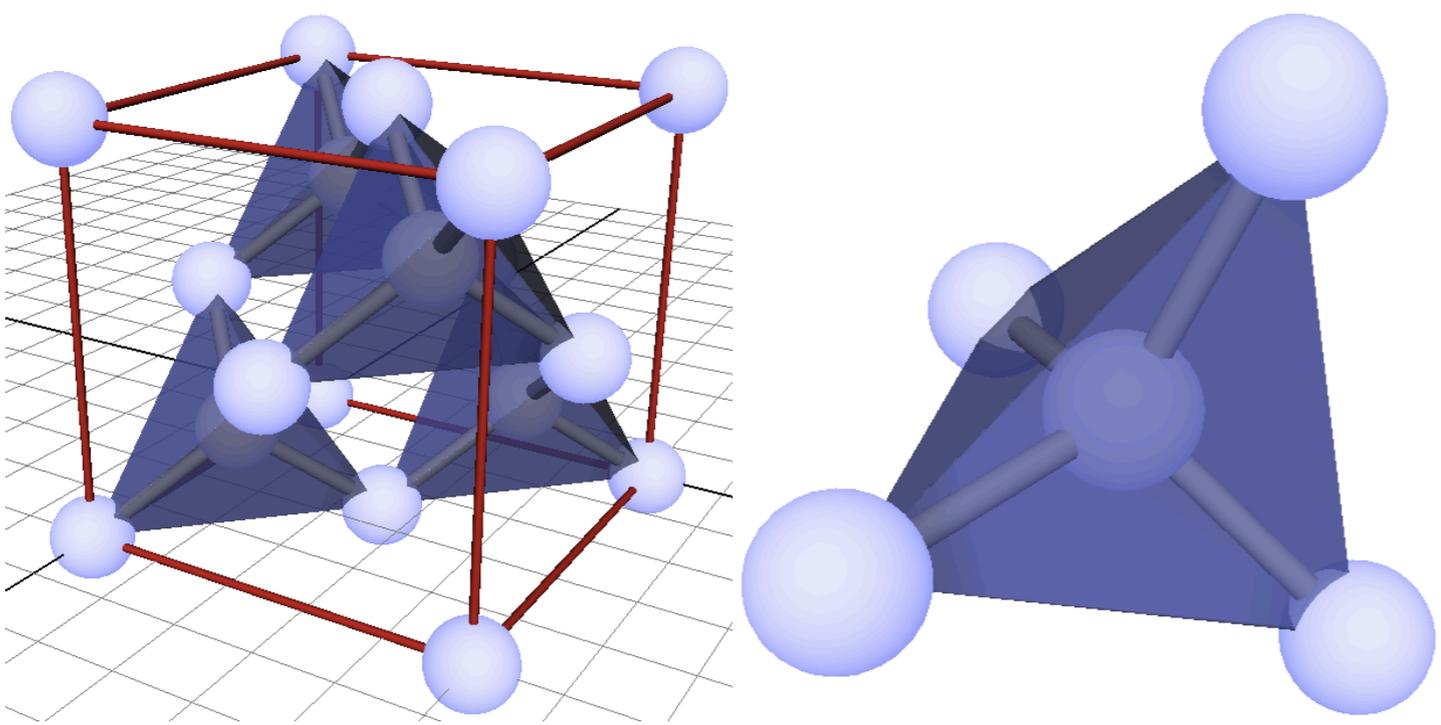
Fig.5  $\gamma/\epsilon$  stabilizing parameter of alloying elements at 500°K

# stacking fault in diamond [I]



dual fcc

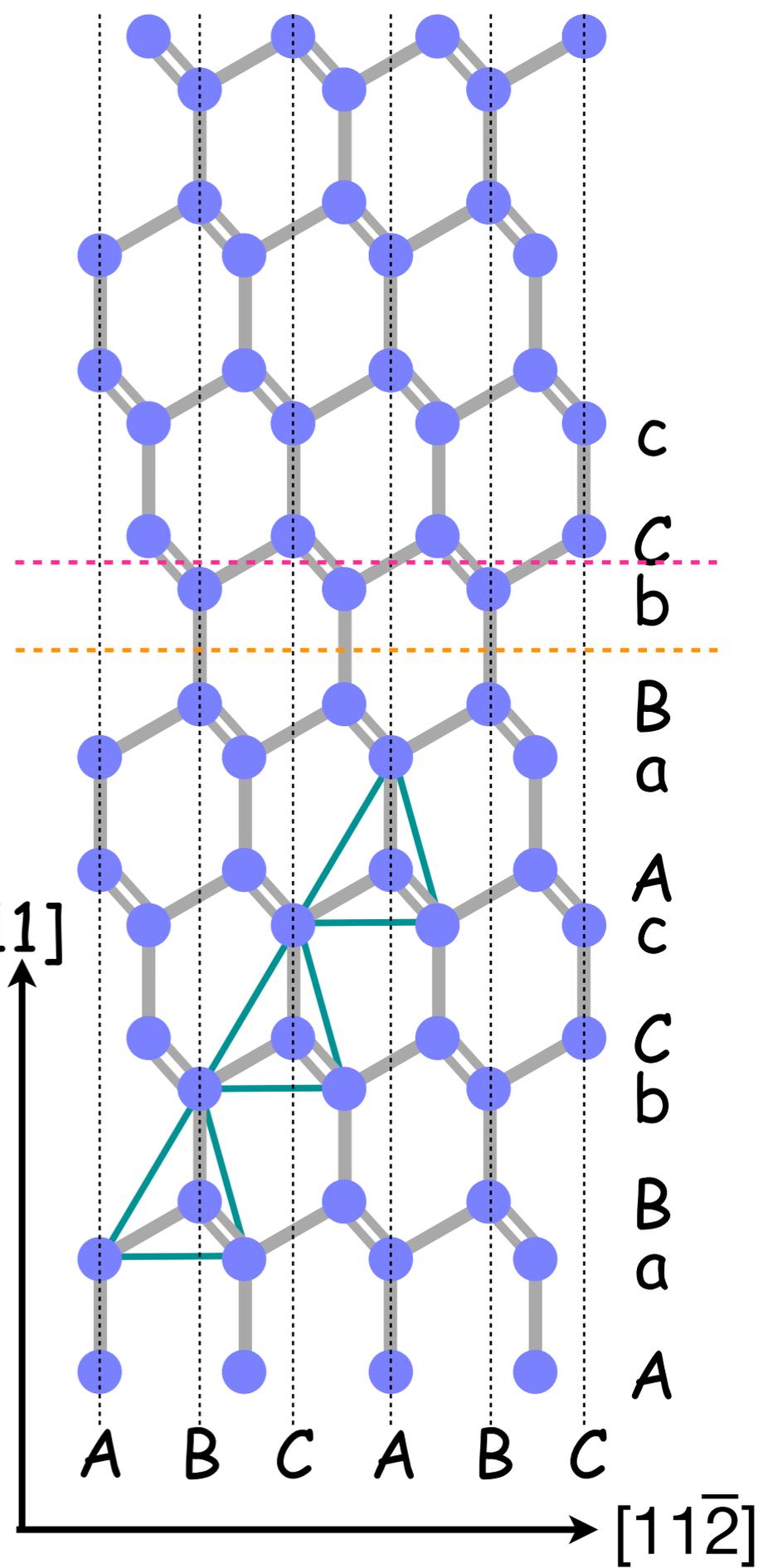
diamond



diamond

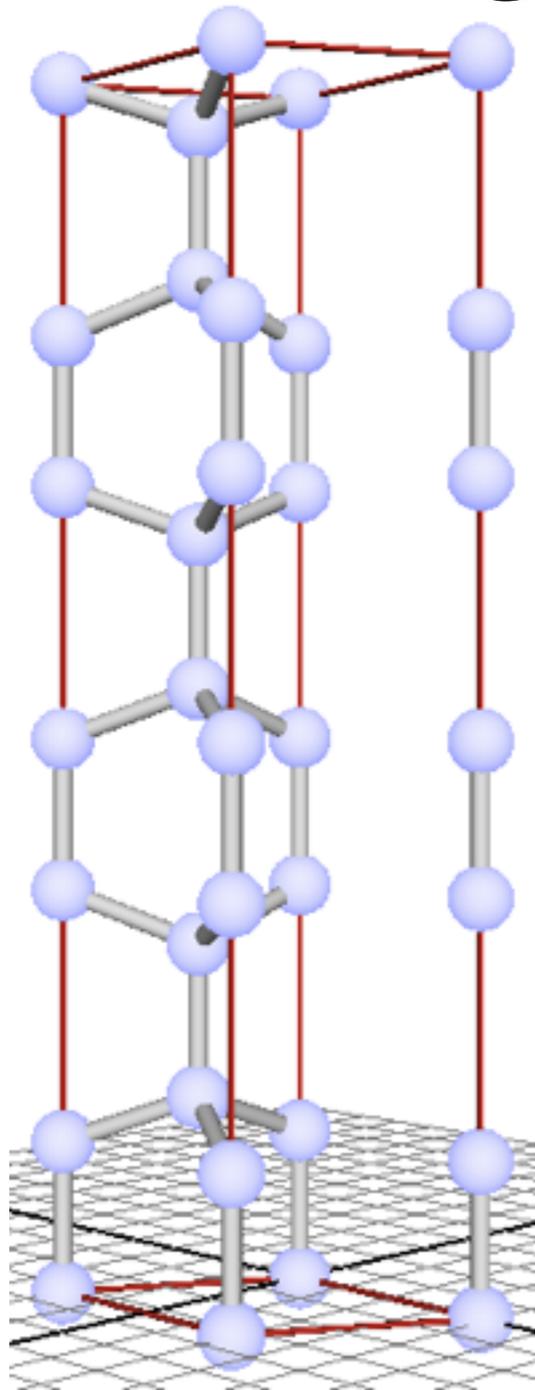
tetragonal

glide-set  
shuffle-set





# Calculation I



2H

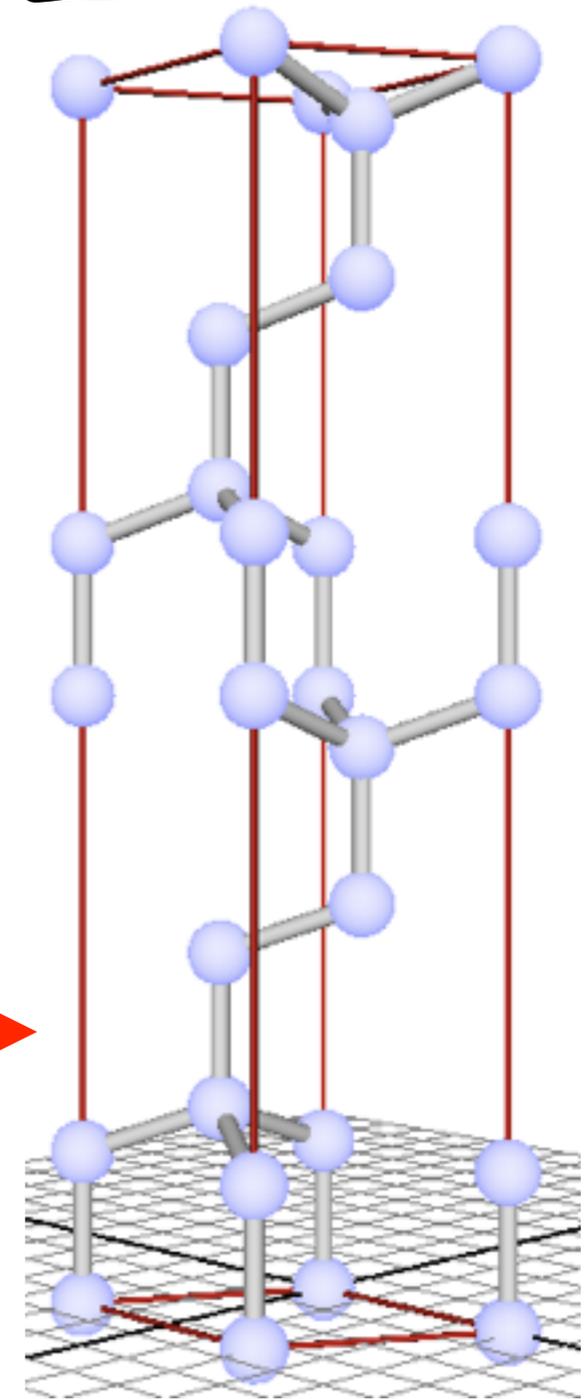
- 2H
- $1 \times 1 \times 3$
- 3C
- $1 \times 1 \times 2$ .

→ 6 layers



structure energy  
difference between 2H  
and 3C

$$\Delta E = E_{2H} - E_{3C}$$

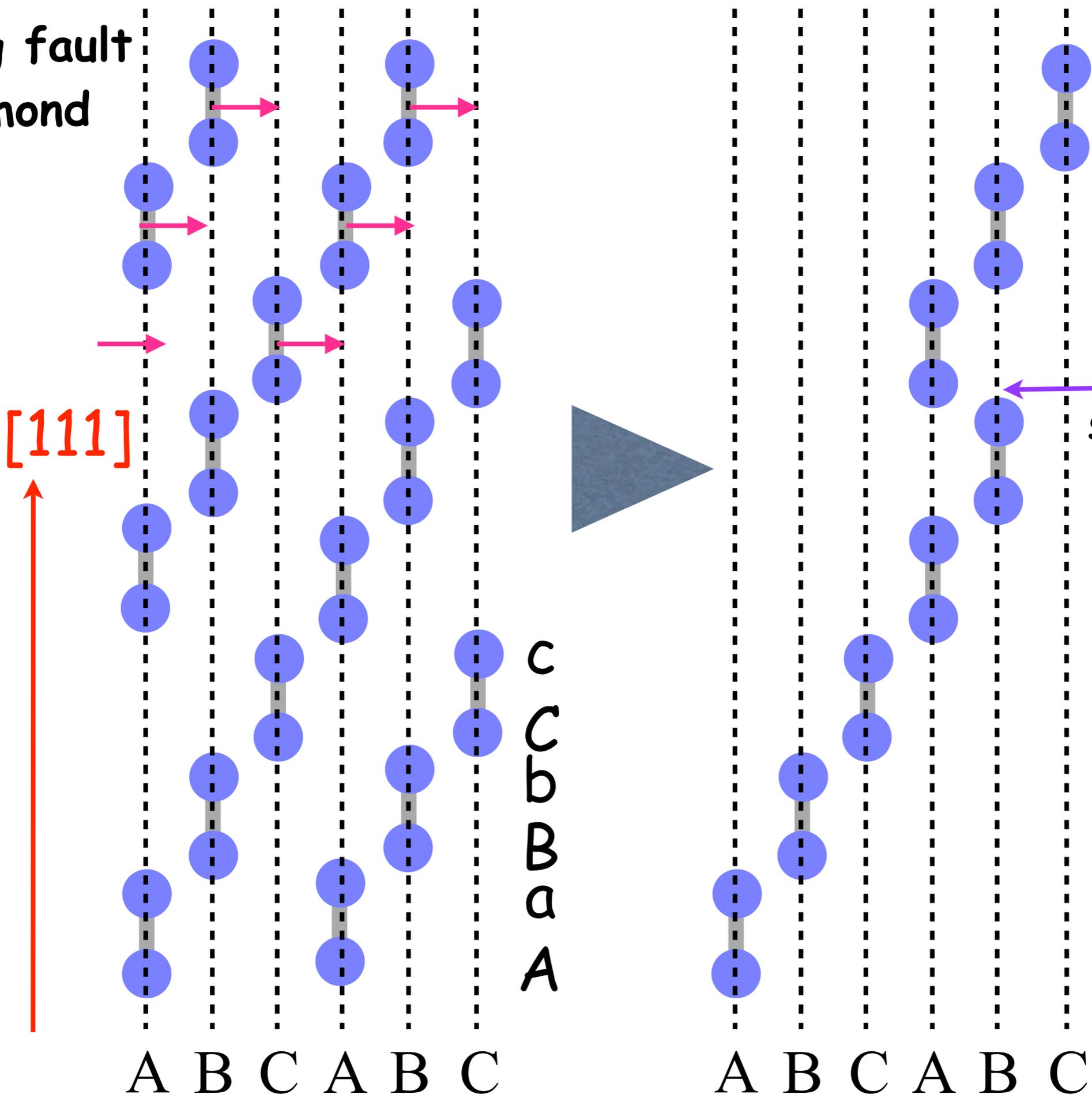


3C

# Results I

dopant	structure energy difference	$\Delta E$ [eV]
non-doped	$E_{2H-Si} - E_{3C-Si}$	0.1331
P	$E_{2H-Si(P)} - E_{3C-Si(P)}$	0.0632
B	$E_{2H-Si(B)} - E_{3C-Si(B)}$	0.0871

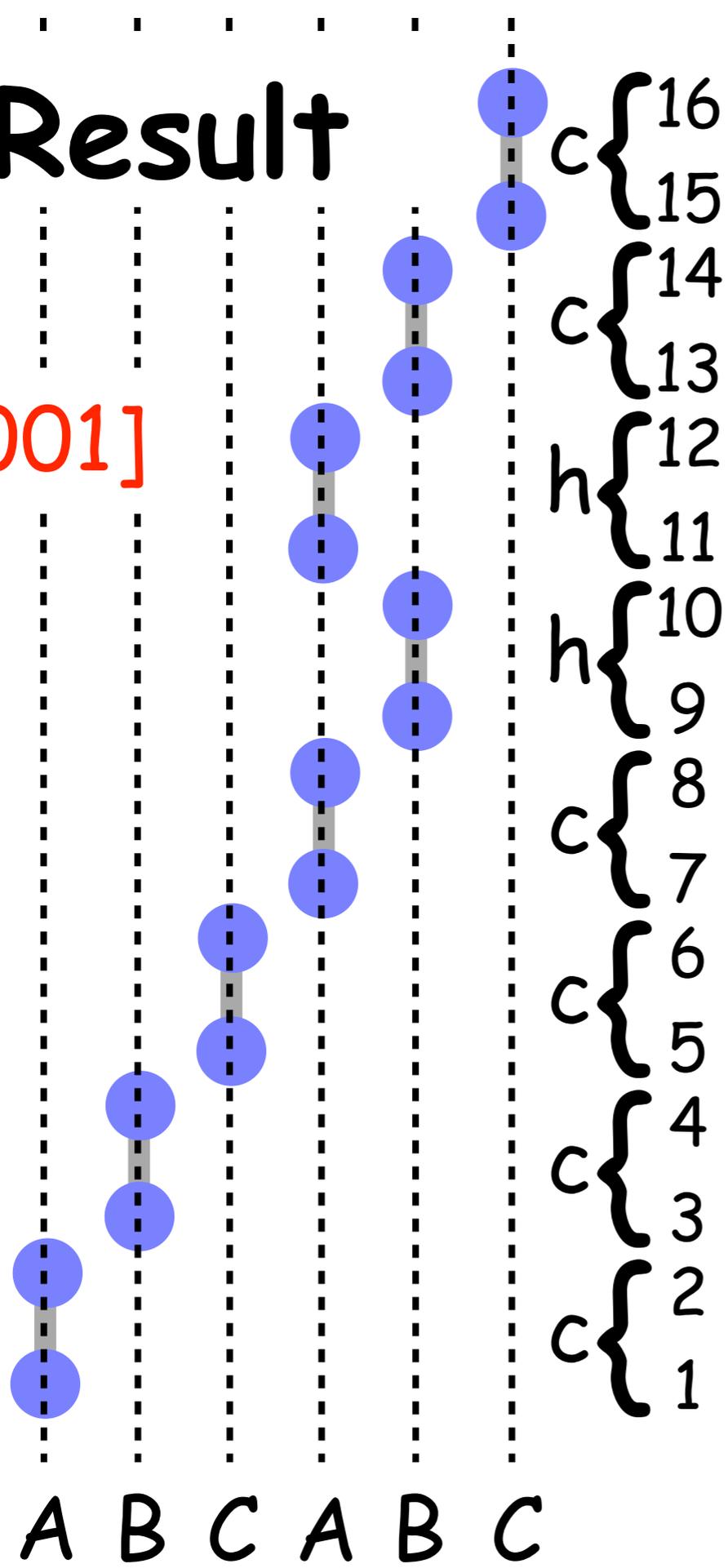
# Stacking fault in diamond



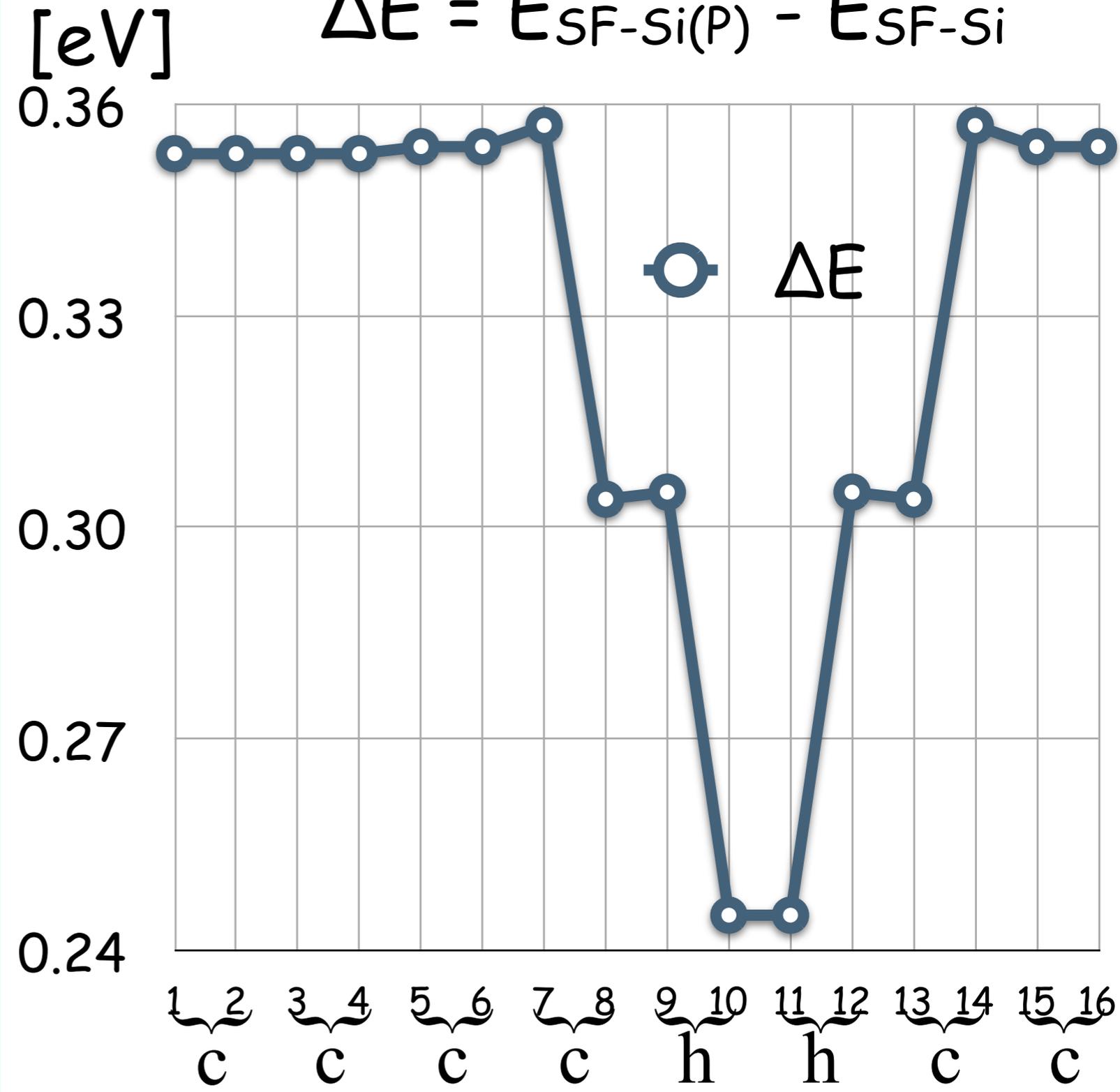
Intrinsic stacking fault

# Result

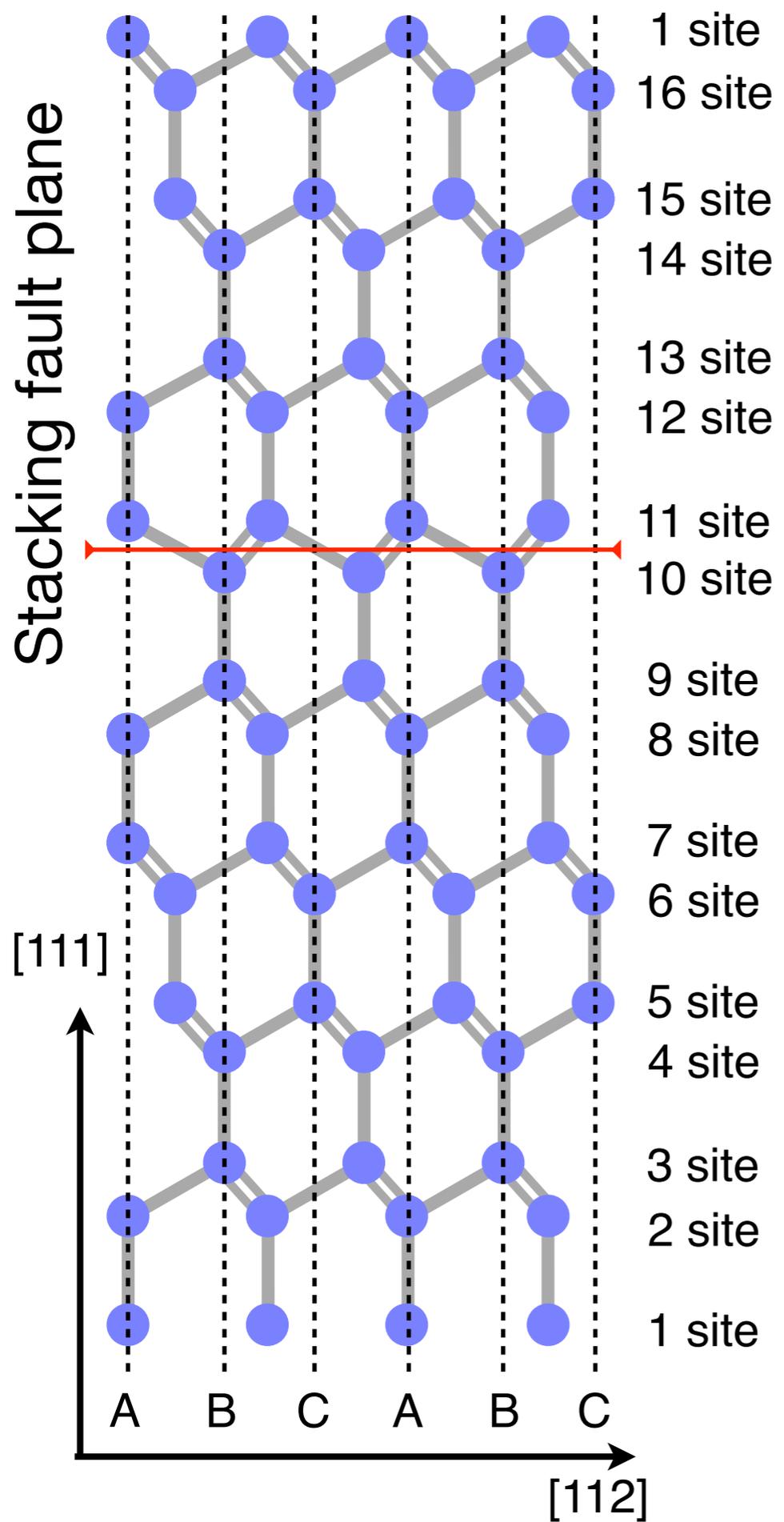
[0001]



$$\Delta E = E_{SF-Si(P)} - E_{SF-Si}$$

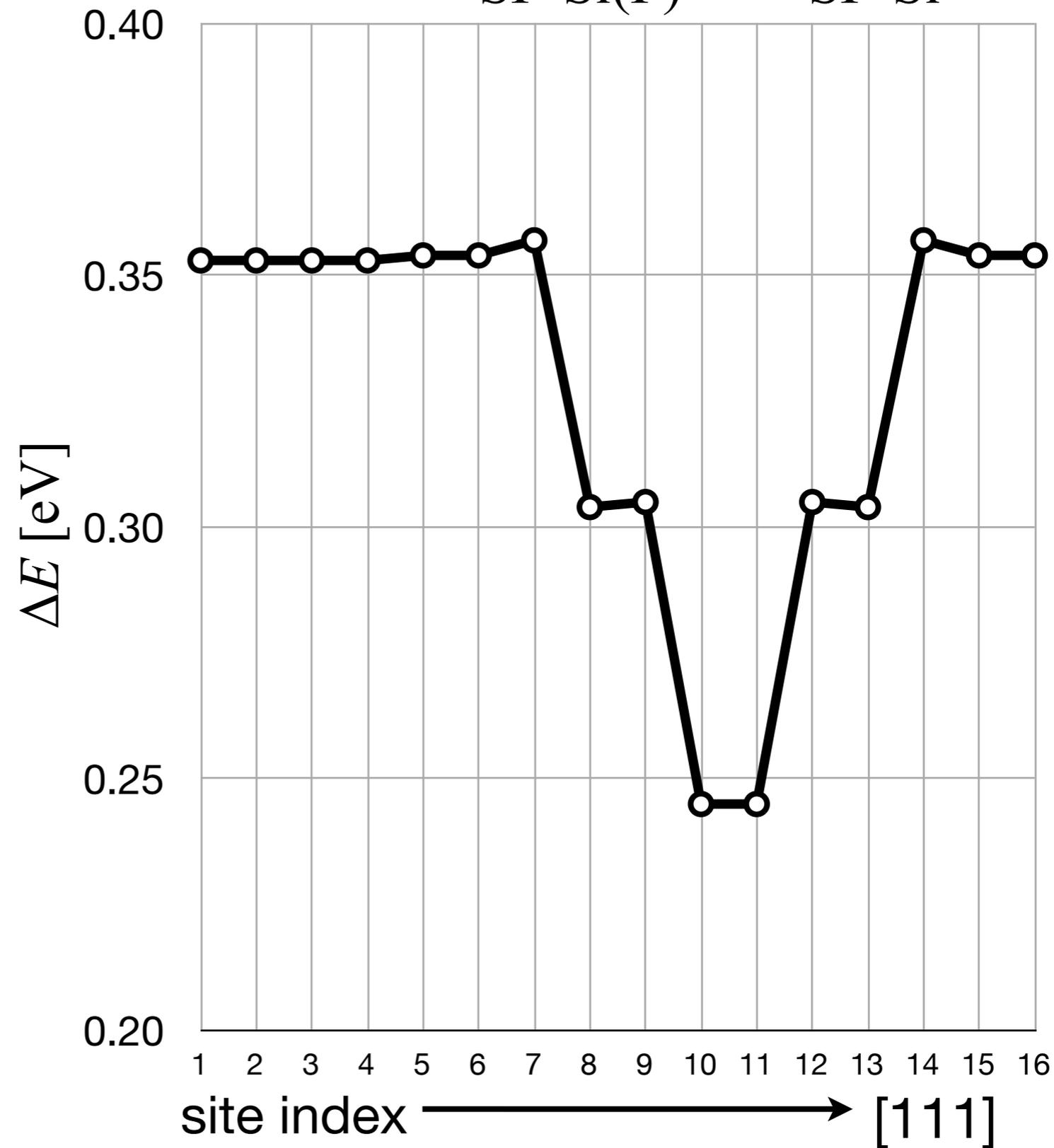


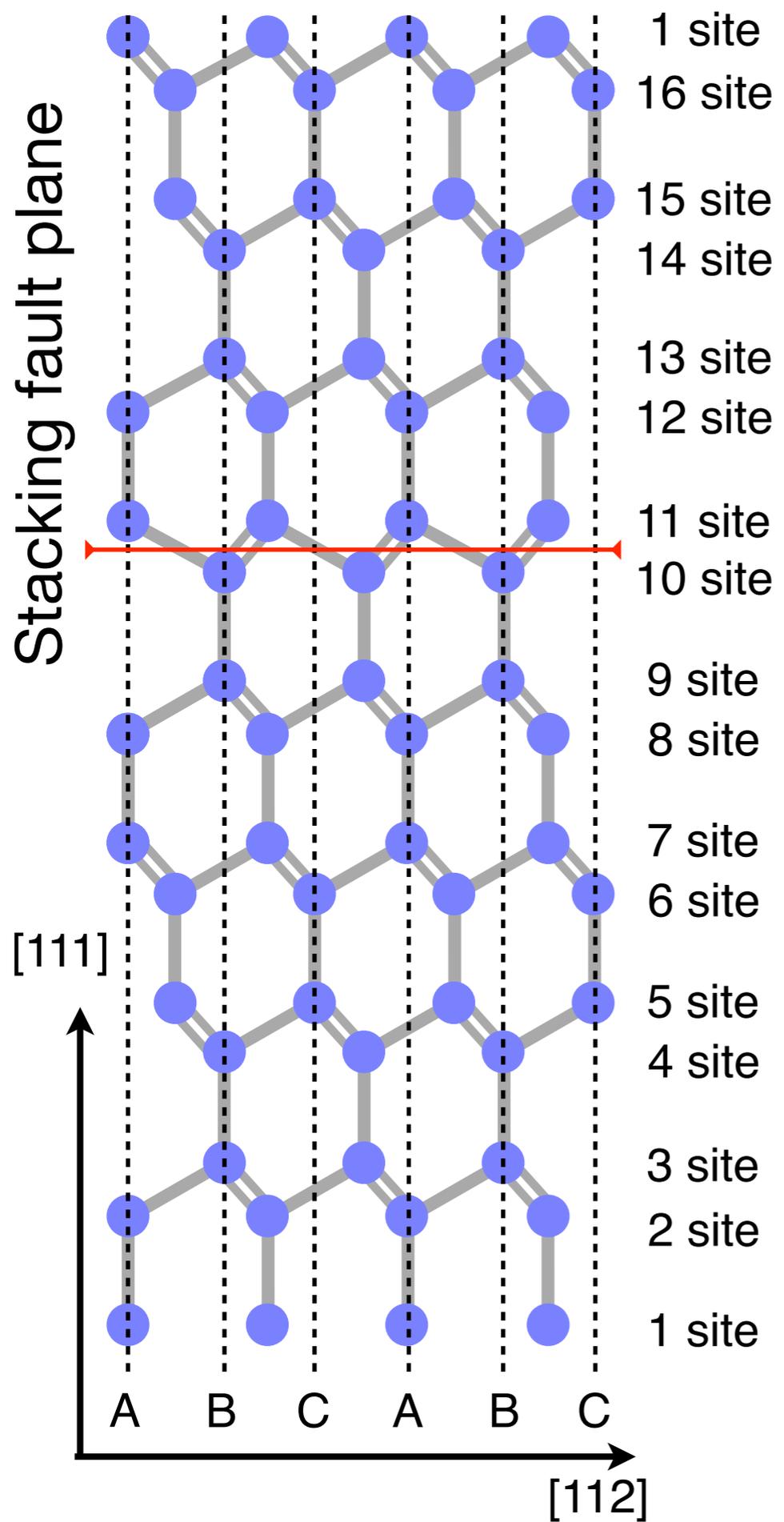
Results indicate P prefers in h-sequence [0001]



# Si+P

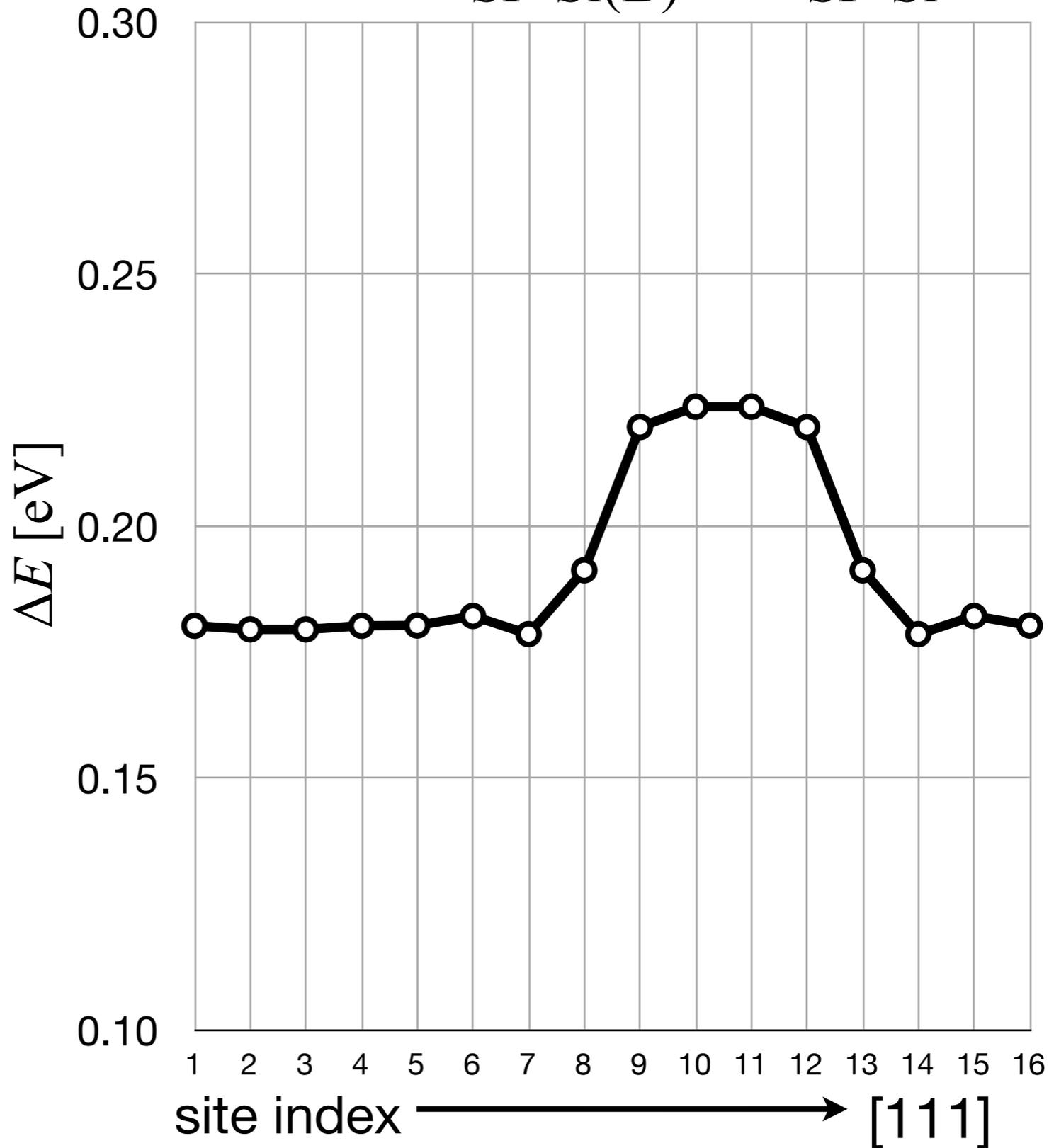
$$\Delta E = E_{\text{SF-Si(P)}} - E_{\text{SF-Si}}$$





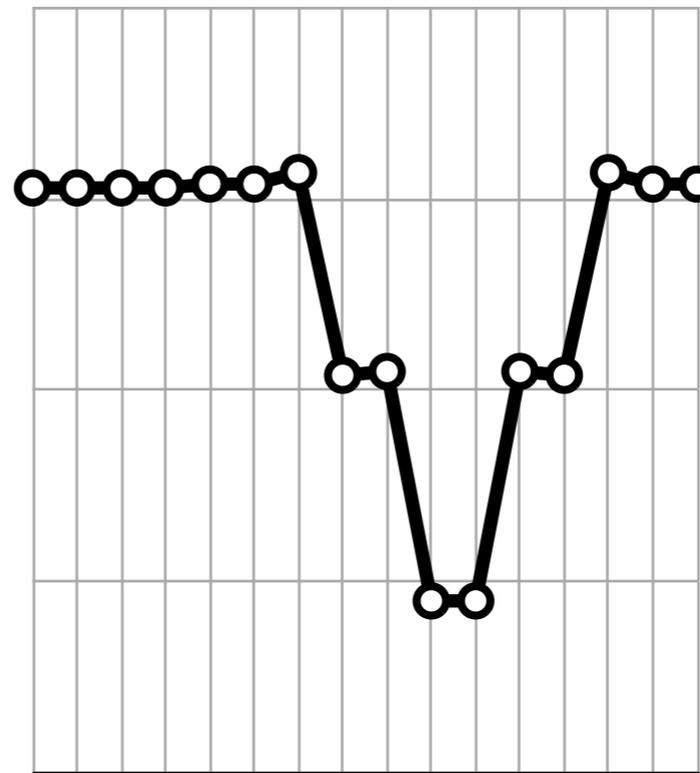
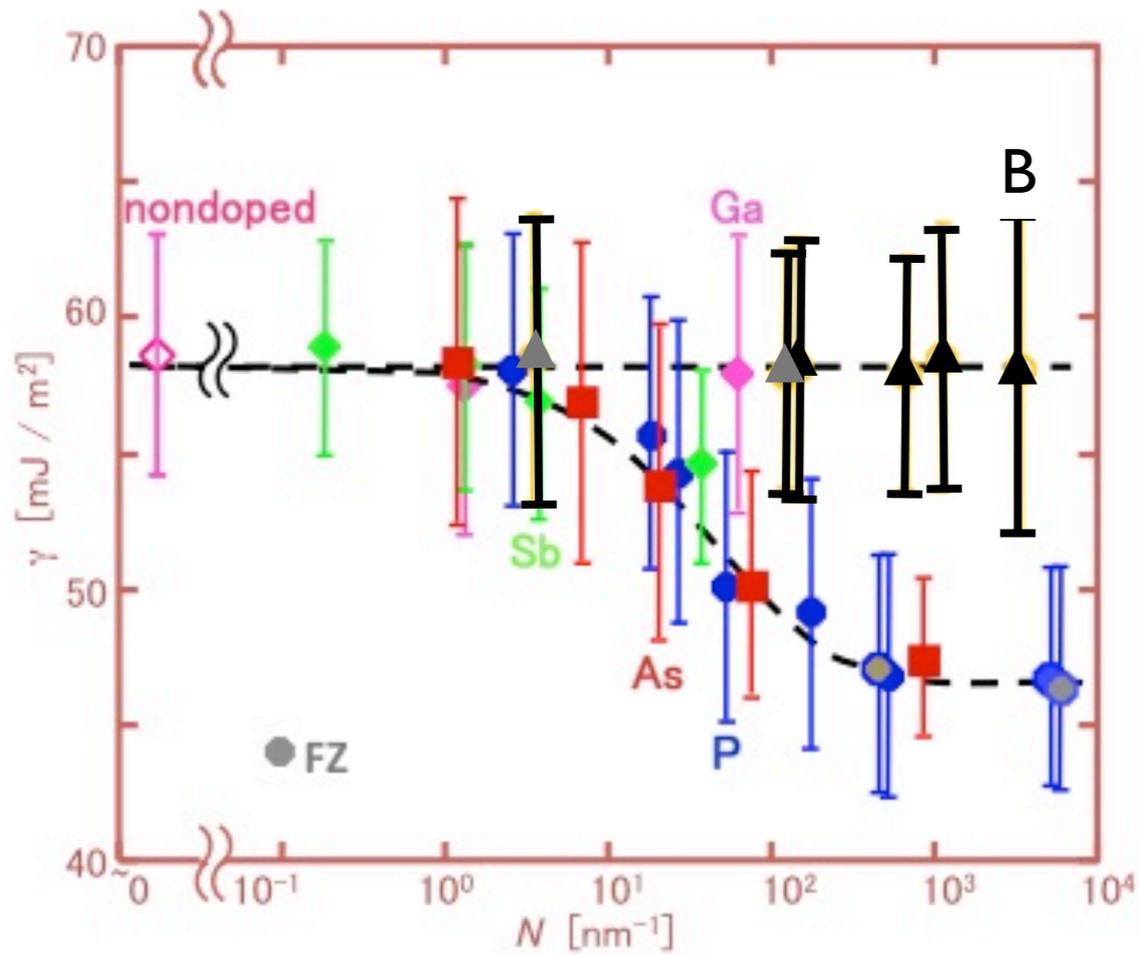
# Si+B

$$\Delta E = E_{\text{SF-Si(B)}} - E_{\text{SF-Si}}$$

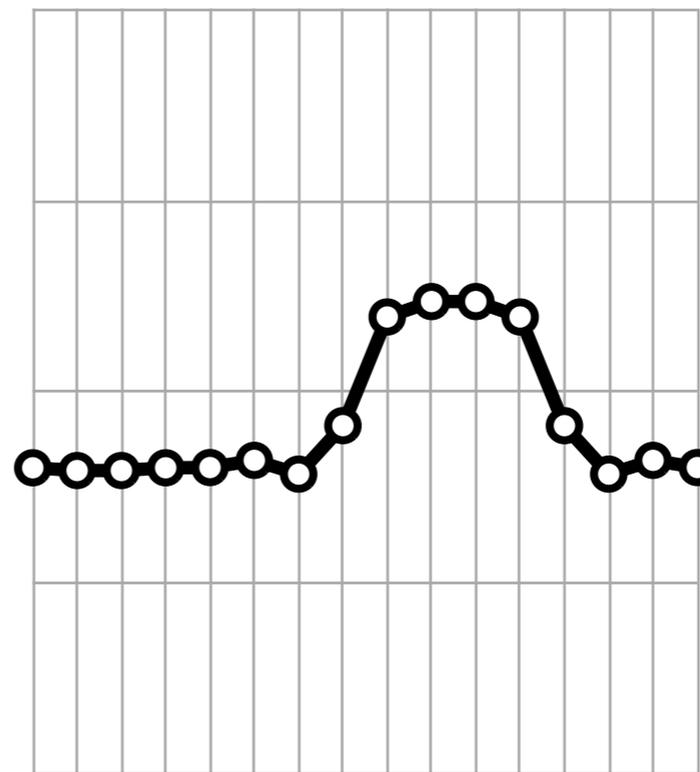


# Results II

- Consistency
- ▶ P: S.F. Energy decrease
- ▶ B: No change



P-doped Si



B-doped Si