Podstawy Programowania w JĄzyku C

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(a)

Outline
Bulk materials parametriazation
Formation energy
NEB method
Phonon calculation
Summarizing

Outline

1. Bulk materials parametriazation
   - GaN
   - InN
   - AlN

2. Formation energy

3. NEB method
   - parametrs

4. Phonon calculation

5. Summarizing

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GaN
InN
AlN

Wurtzite GaN

Material	a, Å	Δa	c/a
GaN	3.186	-	1.61

Refernce

1:

2:

Wurtzite InN

Wurtzite AlN

Block

Parametrs

parametrs

Nudgest Elastic Bands method

parametrs

Images

12 Images

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Phonon calculation

Thank u =)