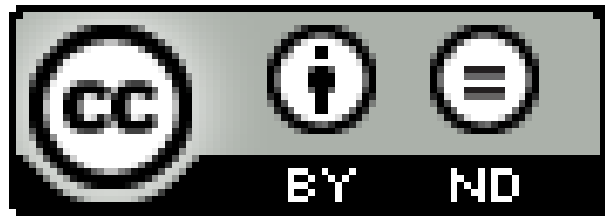
T

x


BY
ND

σ_i

-1

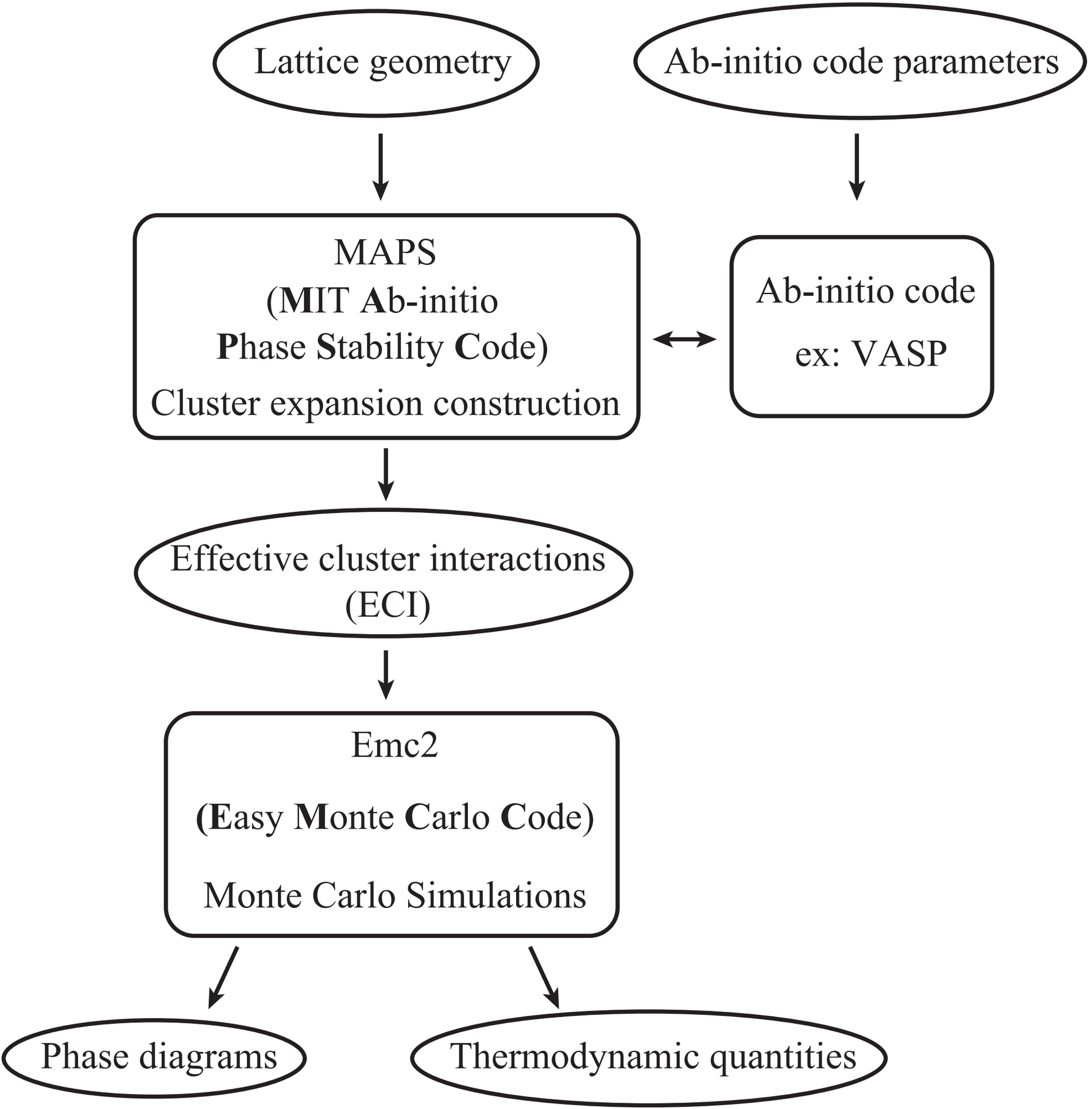
σ

$$E(\sigma) = \sum_{\alpha} m_{\alpha} J_{\alpha} \left\langle \prod_{i \in \alpha'} \sigma_i \right\rangle$$

α

$$m_\alpha$$

$E\left(\sigma\right)$


Lattice geometry
Ab-initio code parameters
MAPS
(MIT Ab-initio
Phase Stability Code)
Cluster expansion construction
Ab-initio code
ex: VASP
Effective cluster interactions
(ECI)
Emc2
(Easy Monte Carlo Code)
Monte Carlo Simulations
Phase diagrams
Thermodynamic quantities

a

b

c

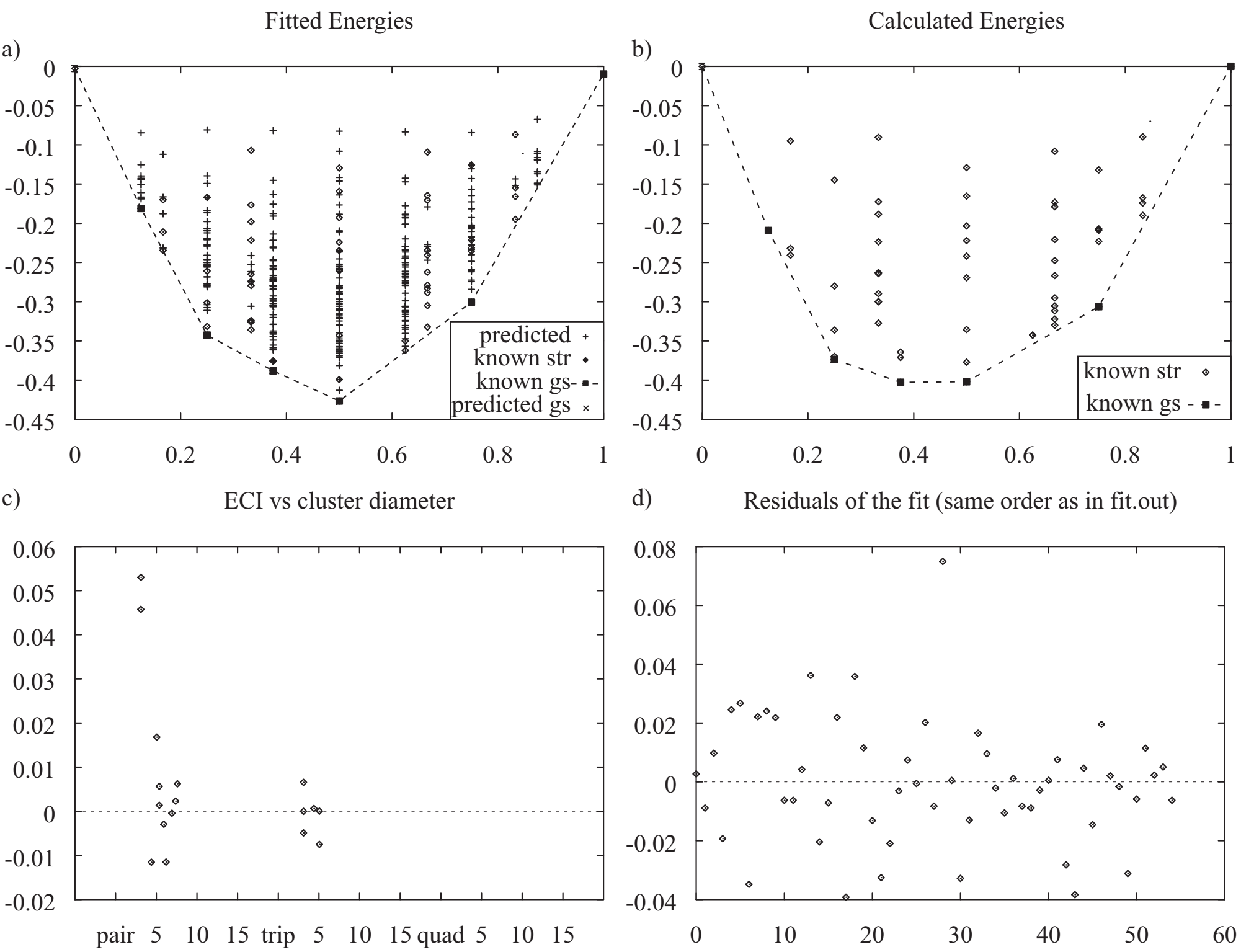
k

n

S

$$\mathrm{CV}=\left(\frac{1}{n}\sum_{i=1}^{n}\left(E_i-\hat{E}_{(i)}\right)^2\right)^{1/2}$$

$(n-1)$

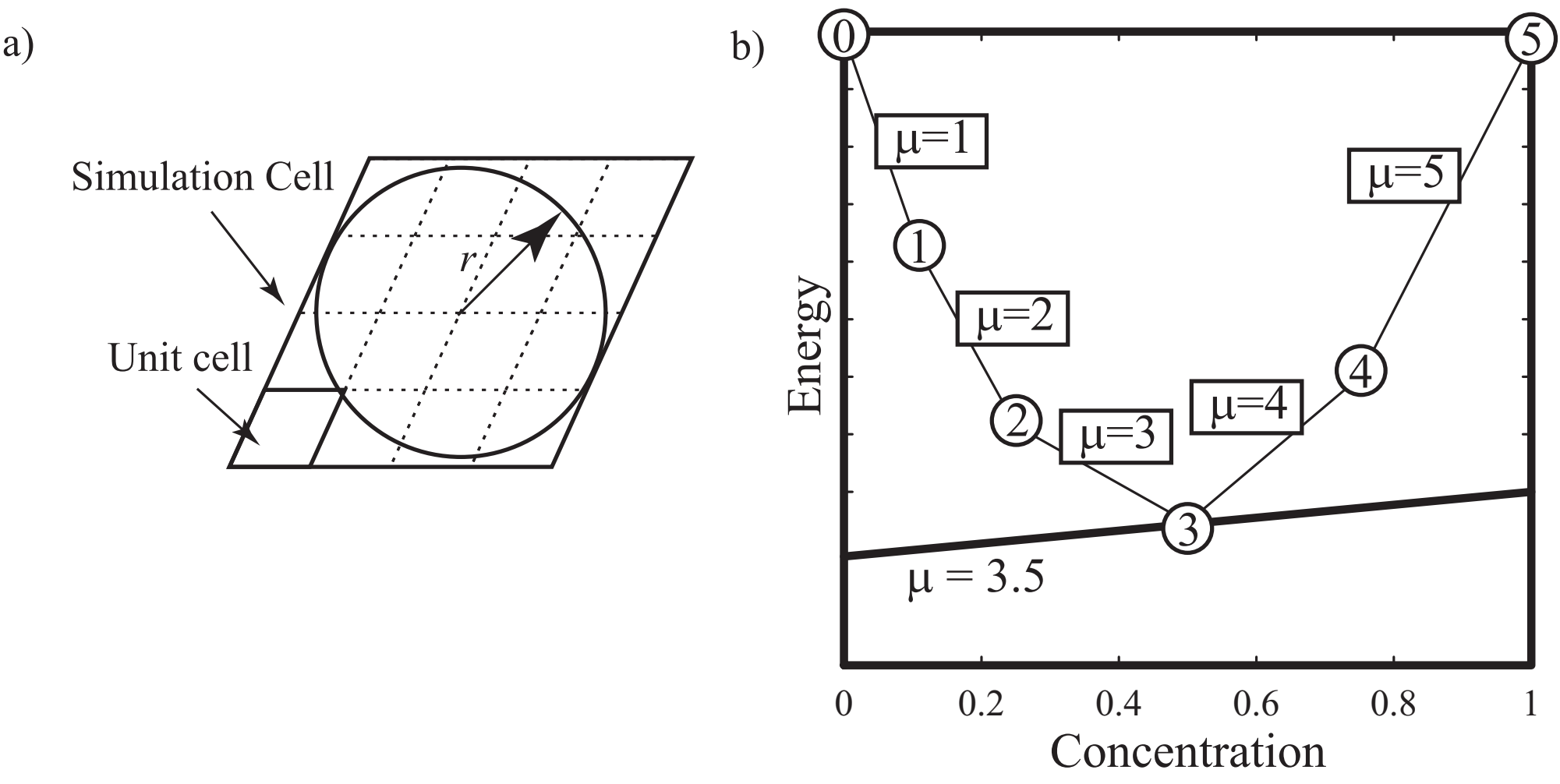

Fitted Energies
a)
predicted
known str
known gs
predicted gs
Calculated Energies
b)
known str
known gs
c)
ECI vs cluster diameter
pair 5 10 15 trip 5 10 15 quad 5 10 15
d)
Residuals of the fit (same order as in fit.out)

$G - 1$

n_1

n_2

γ


a)
Simulation Cell
Unit cell
r
b)
0
1
2
3
4
5
μ=1
μ=2
μ=3
μ=4
μ=5
μ = 3.5
Energy
0
0.2
0.4
0.6
0.8
1
Concentration

n_{eq}

n_{avg}

T_0

T_1

ΔT

$\Delta(1/T)$

$T_0 = 0$

k_B

8.617×10^{-5}

3.0

2

3

4.0

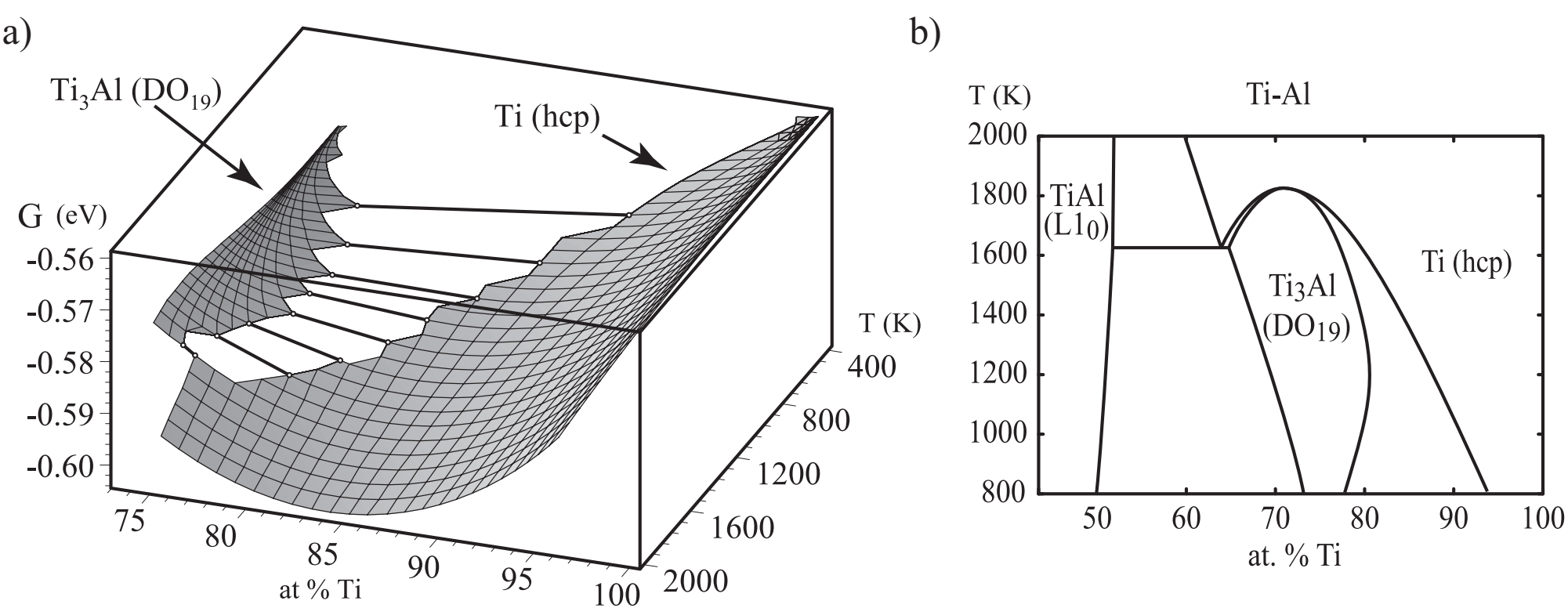
μ_0

μ_1

μ

1

1.5


a)
Ti3Al (DO19)
Ti (hcp)
G (eV)
-0.56
-0.57
-0.58
-0.59
-0.60
75
80
85
90
95
100
at % Ti
T (K)
400
800
1200
1600
2000
b)
T (K)
Ti-Al
2000
1800
1600
1400
1200
1000
800
TiAl
(L10)
Ti3Al
(DO19)
Ti (hcp)
50
60
70
80
90
100
at. % Ti

25

5×10^{-3}

$$\phi = G - \mu x$$

E

$1-x$

x

2

2

3

$E - \mu x$