From Atoms to Materials: Predictive Theory and Simulations

Week 5 – Homework solution 3

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Charge equilibration Q.1.1

- Di-atomic molecule

$$E(\{q_i\}) = \sum_{i<j} \frac{q_i q_j}{R} + \sum_i \left(\chi_i q_i + \frac{1}{2} H_i q_i^2 \right)$$

Coulomb

EA / IP

Charge equilibration Q.1.1

- Di-atomic molecule

$$E(\{q_i\}) = \sum_{i<j} \frac{q_i q_j}{R} + \sum_i \left(\chi_i q_i + \frac{1}{2} H_i q_i^2 \right)$$

Coulombic interaction

Total electrostatic: EA and IP

$$E(\{q_i\}) = 14.4 \frac{q_\alpha q_\beta}{R} + \chi_\alpha q_\alpha + \chi_\beta q_\beta + \frac{1}{2} H_\alpha q_\alpha^2 + \frac{1}{2} H_\beta q_\beta^2$$

Charge equilibration Q.1.2

- Di-atomic molecule

$$E(\{q_i\}) = 14.4\frac{q_\alpha q_\beta}{R} + \chi_\alpha q_\alpha + \chi_\beta q_\beta + \frac{1}{2}H_\alpha q_\alpha^2 + \frac{1}{2}H_\beta q_\beta^2$$

- Chemical potential

$$\mu = \frac{\partial E}{\partial q_\alpha}$$

Charge equilibration Q.1.2

- Di-atomic molecule

$$E(\{q_i\}) = 14.4\frac{q_\alpha q_\beta}{R} + \chi_\alpha q_\alpha + \chi_\beta q_\beta + \frac{1}{2}H_\alpha q_\alpha^2 + \frac{1}{2}H_\beta q_\beta^2$$

- Chemical potential

$$\mu = \frac{\partial E(\{q_i\})}{\partial q_\alpha}$$

$$\rightarrow \boxed{\mu = 14.4\frac{q_\beta}{R} + \chi_\alpha + H_\alpha q_\alpha}$$

Charge equilibration Q.1.3

- Di-atomic molecule

$$E(\{q_i\}) = 14.4\frac{q_\alpha q_\beta}{R} + \chi_\alpha q_\alpha + \chi_\beta q_\beta + \frac{1}{2}H_\alpha q_\alpha^2 + \frac{1}{2}H_\beta q_\beta^2$$

- Neutral total charge $q_\alpha = -q_\beta$

Charge equilibration Q.1.3

- Di-atomic molecule

$$E(\{q_i\}) = 14.4\frac{q_\alpha q_\beta}{R} + \chi_\alpha q_\alpha + \chi_\beta q_\beta + \frac{1}{2}H_\alpha q_\alpha^2 + \frac{1}{2}H_\beta q_\beta^2$$

- Neutral total charge $q_\alpha = -q_\beta$

$$E(\{q_i\}) = -14.4\frac{q_\alpha^2}{R} + \chi_\alpha q_\alpha - \chi_\beta q_\alpha + \frac{1}{2}H_\alpha q_\alpha^2 + \frac{1}{2}H_\beta q_\alpha^2$$

$$\frac{\partial E}{\partial q_\alpha} = 0$$

Charge equilibration Q.1.3

- Di-atomic molecule

$$E(\{q_i\}) = 14.4\frac{q_\alpha q_\beta}{R} + \chi_\alpha q_\alpha + \chi_\beta q_\beta + \frac{1}{2}H_\alpha q_\alpha^2 + \frac{1}{2}H_\beta q_\beta^2$$

- Neutral total charge $q_\alpha = -q_\beta$

$$E(\{q_i\}) = -14.4\frac{q_\alpha^2}{R} + \chi_\alpha q_\alpha - \chi_\beta q_\alpha + \frac{1}{2}H_\alpha q_\alpha^2 + \frac{1}{2}H_\beta q_\alpha^2$$

$$\frac{\partial E(\{q_i\})}{\partial q_\alpha} = 0 \Leftrightarrow q_\alpha = \frac{\chi_\beta - \chi_\alpha}{H_\alpha + H_\beta - 2\frac{14.4}{R}}$$

Charge equilibration

Q.1.4

- Di-atomic molecule NaCl ✓

$$q_{Na} = \frac{\chi_{Cl} - \chi_{Na}}{H_{Na} + H_{Cl} - 2\frac{14.4}{R}}$$

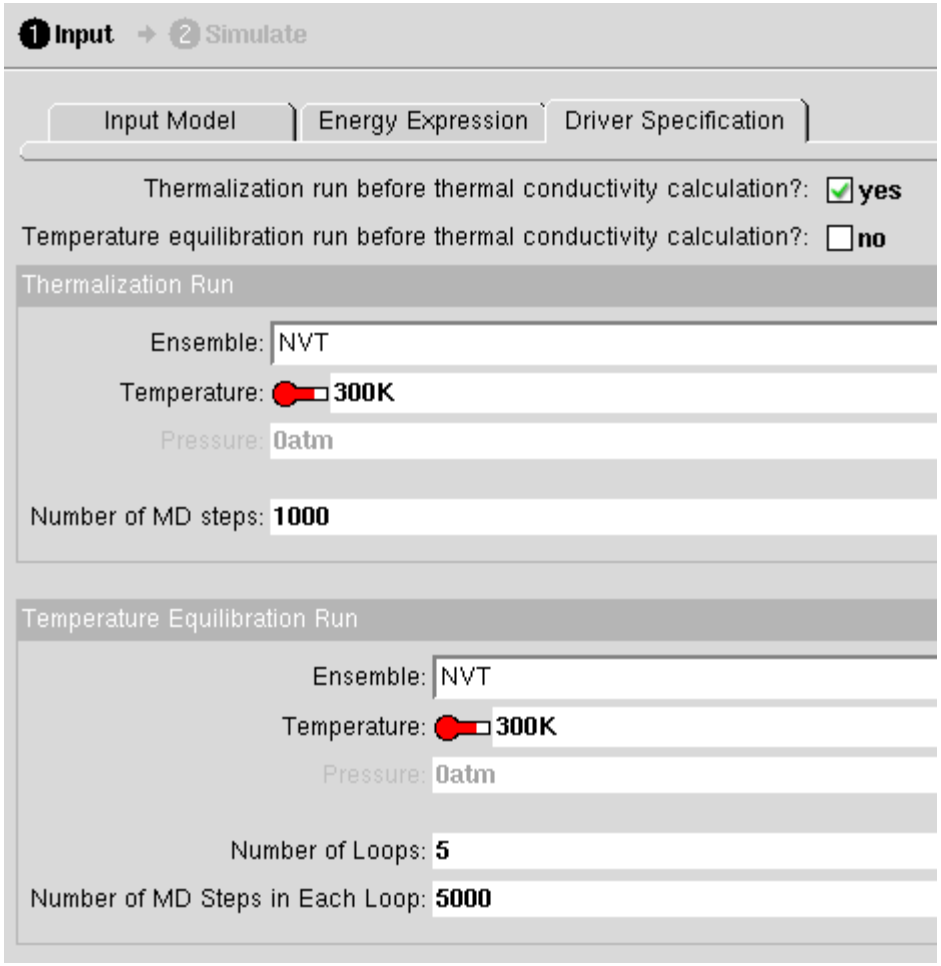
$q_{Na} = 0.92\,e$

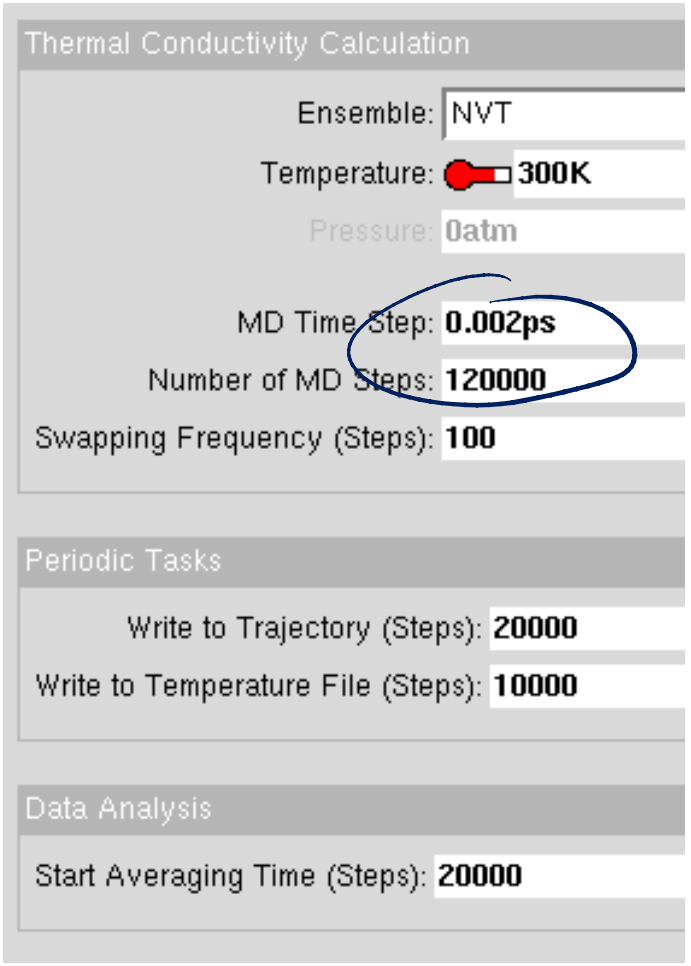
Thermal conductivity

Q.2.1

- MD simulation

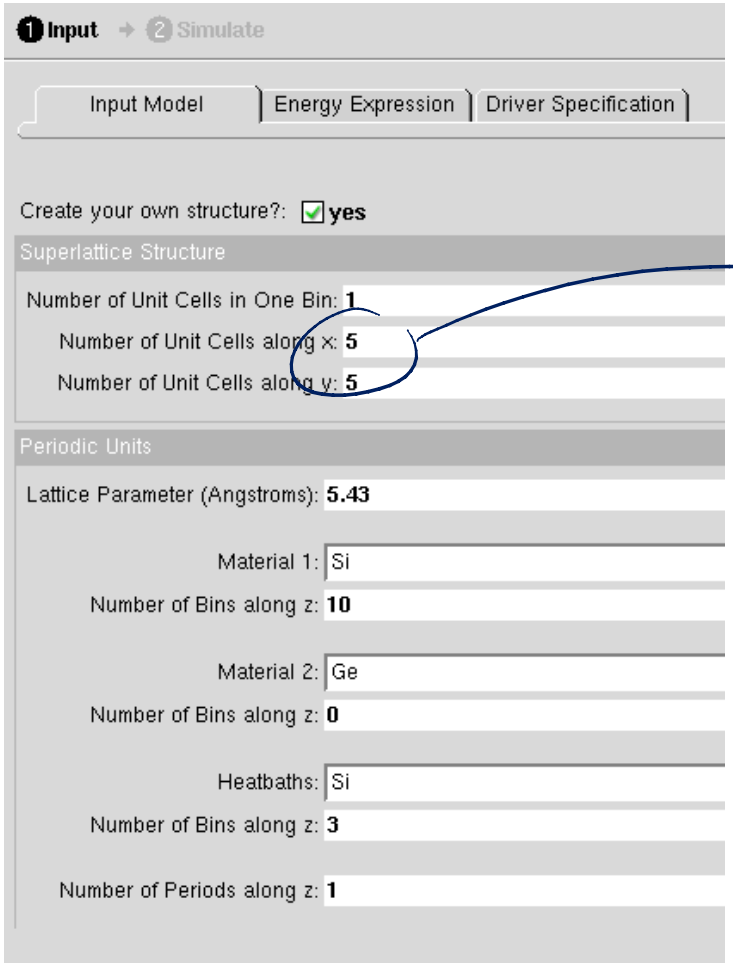
$t = 0.002 \times 120{,}000 = 240\ ps$





Thermal conductivity Q.2.2

- MD simulation

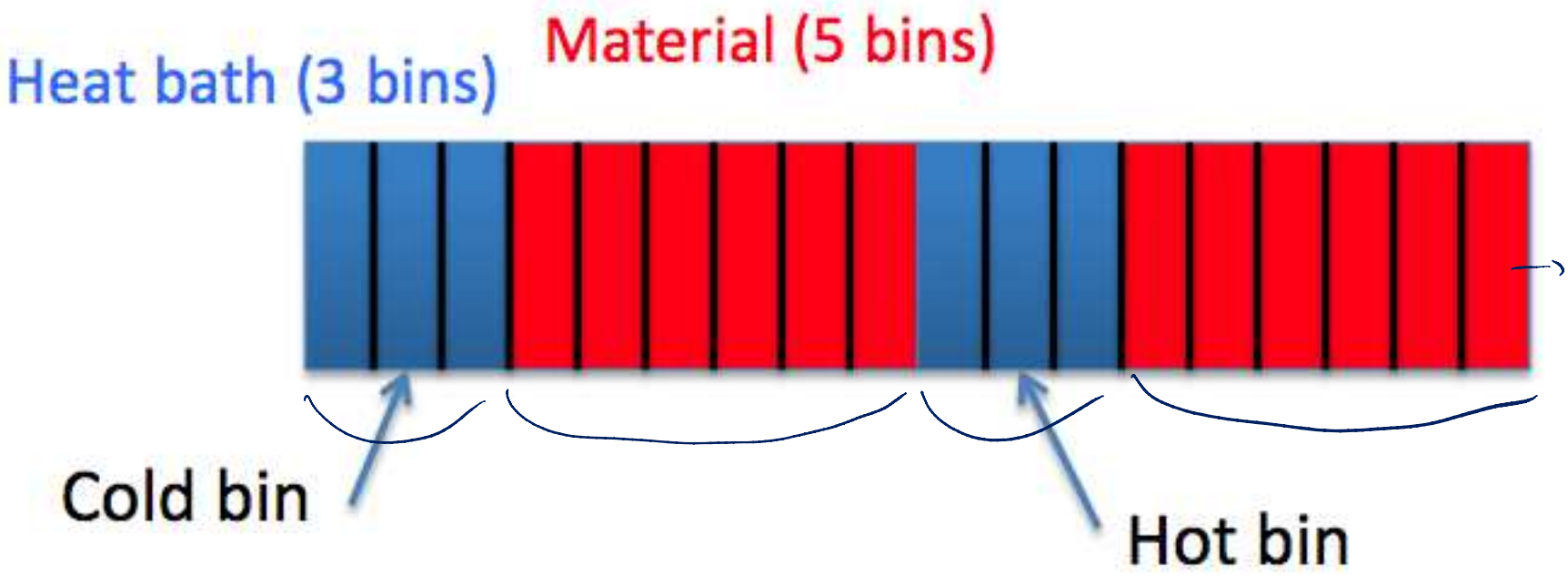


$L_{x,y} = 5 \times 5.43$

$= 27.15$ Å

Thermal conductivity Q.2.3

- MD simulation



- Simulation transport direction (10 bins)

$L = (10+3) \times 2 \times 5.43 = 141.18$ Å

Thermal conductivity Q.2.4

- MD simulation

Result: Thermal Conductivity — 3 bins

```
Thermal Conductivity including Material and Contacts: 1.65454 (W/mK)
Material Thermal Conductivity: 2.47298 (W/mK) from layer 3 ~ 5
KE: 4030.56000 Kcal/mol
Lx: 29.48301 Angstroms
Ly: 29.48168 Angstroms
Time: 200.00000 ps
Total Bin Number: 12
Number of Heatbath: 3
```

Thermal conductivity increases
Limiting the mean free path of phonons

Result: Thermal Conductivity — 5 bins

```
Thermal Conductivity including Material and Contacts: 2.18315 (W/mK)
Material Thermal Conductivity: 2.58948 (W/mK) from layer 3 ~ 7
KE: 4054.77630 Kcal/mol
Lx: 29.48602 Angstroms
Ly: 29.48528 Angstroms
Time: 200.00000 ps
Total Bin Number: 16
Number of Heatbath: 3
```

Result: Thermal Conductivity — 10 bins

```
Thermal Conductivity including Material and Contacts: 3.52272 (W/mK)
Material Thermal Conductivity: 5.40600 (W/mK) from layer 3 ~ 12
KE: 4019.45450 Kcal/mol
Lx: 29.49334 Angstroms
Ly: 29.49295 Angstroms
Time: 200.00000 ps
Total Bin Number: 26
Number of Heatbath: 3
```