LJ model と KW model

LJ; $T_{red}(x) = x T_{c1} + (1-x) T_{c2} + x(1-x)\xi$

KW; $T_{red}(x) = x^2 T_{c1} + (1-x)^2 T_{c2} + 2\gamma_T x(1-x) T_{c12,KW}$

$(\beta_T = 1)$ $\quad T_{c12,KW} = \sqrt{T_{c1} T_{c2}}$

$\gamma_T = \dfrac{\xi + T_{c1} + T_{c2}}{2 T_{c12,KW}}$ とおけば、

KW; $T_{red}(x) = x^2 T_{c1} + (1-x)^2 T_{c2} + x(1-x)(\xi + T_{c1} + T_{c2})$

$= x^2 T_{c1} + (1-x)^2 T_{c2} + x(1-x)(T_{c1} + T_{c2})$

$\quad + x(1-x)\xi$

$= x T_{c1} + (1-x) T_{c2} + x(1-x)\xi \longrightarrow$ LJ model

LJ

$$T_{red}(x) = x\,T_{c1} + (1-x)T_{c2} + x(1-x)\,T_{c12,LJ}$$

KW

$$T_{red}(x) = x^2 T_{c1} + (1-x)^2 T_{c2} + 2\gamma_T x(1-x)\,T_{c12,KW}$$

$$= x^2 T_{c1} + (1-2x+x^2)T_{c2} + 2\gamma_T x(1-x)\,T_{c12,KW}$$

$$T_{red}(x) = x^2 T_{c1} + (1-x)^2 T_{c2} + 2x(1-x)\,T_{c12}$$

$$T_{c12} = \frac{T_{c1}+T_{c2}}{2}$$

$$T_{red}(x) = x^2 T_{c1} + (1-x)^2 T_{c2} + x(1-x)(T_{c1}+T_{c2})$$

$$= x^2 T_{c1} + (1-2x+x^2)T_{c2} + (x-x^2)(T_{c1}+T_{c2})$$

$$= x^2 T_{c1} + T_{c2} - 2x\,T_{c2} + x^2 T_{c2} + x\,T_{c1} + x\,T_{c2} - x^2 T_{c1} - x^2 T_{c2}$$

$$= x\,T_{c1} + T_{c2} - x\,T_{c2}$$

$$= x\,T_{c1} + (1-x)T_{c2}$$

$$T_{c12,KW} = \frac{\sqrt{T_{c1}T_{c2}}}{\frac{T_{c1}+T_{c2}}{2}}, \qquad \gamma_T = \frac{T_{c1}+T_{c2}}{2}$$

$$= \sqrt{T_{c1}T_{c}} \qquad \gamma_T = \frac{(T_{c1}+T_{c2})}{2\sqrt{T_{c1}T_{c2}}}$$

$$T_{c12\,KW} = \sqrt{T_{c1} T_{c2}}$$

$$x^2 T_{c1} + (1-x)^2 T_{c2} + 2\gamma_T x(1-x) T_{c12,KW}.$$

$$\gamma = \frac{T_{c1} + T_{c2}}{2 T_{c12\,KW}}$$

$$= x^2 T_{c1} + (1-x) T_{c2} + x(1-x)(T_{c1} + T_{c2})$$

$$= x T_{c1} + (1-x) T_{c2}$$

$\gamma = \dfrac{\xi + T_{c1} + T_{c2}}{2 T_{c12\,KW}}$ とおけば

$$x^2 T_{c1} + (1-x)^2 T_{c2} + x(1-x)(\xi + T_{c1} + T_{c2})$$

$$= x^2 T_{c1} + (1-x)^2 T_{c2} + x(1-x)(T_{c1} + T_{c2}) + x(1-x)\xi$$

$$= x T_{c1} + (1-x) T_{c2} + x(1-x)\xi.$$