①

$$V_{total} = \sum_{\substack{i,j \\ i<j}} \upsilon_2(i,j) + \sum_{\substack{i,j,k \\ i<j<k}} \upsilon_3(i,j,k)$$

$$* \quad \upsilon_2(r_{ij}) = \varepsilon \cdot f_2\left(\frac{r_{ij}}{\sigma}\right) = \varepsilon \cdot f_2(\bar{r}_{ij})$$

$$f_2(\bar{r}_{ij}) = \begin{cases} A \cdot (B \cdot \bar{r}_{ij}^{-4} - 1) \cdot \exp(\bar{r}_{ij} - a)^{-1} ; & \bar{r}_{ij} < a \\ 0 ; & \bar{r}_{ij} \geq a \end{cases}$$

$$* \quad \upsilon_3(r_i, r_j, r_k) = \varepsilon \cdot f_3\left(\frac{r_i}{\sigma}, \frac{r_j}{\sigma}, \frac{r_k}{\sigma}\right)$$

$$f_3(\bar{r}_i, \bar{r}_j, \bar{r}_k) = h_i(\bar{r}_{ij}, \bar{r}_{ik}, \theta_{jik}) + h_j(\bar{r}_{ji}, \bar{r}_{jk}, \theta_{ijk})$$

$$+ h_k(\bar{r}_{ki}, \bar{r}_{kj}, \theta_{ikj})$$

$$h_i(\bar{r}_{ij}, \bar{r}_{ik}, \theta_{jik}) = \lambda \cdot \exp\left[\gamma(\bar{r}_{ij} - a)^{-1} + \gamma(\bar{r}_{ik} - a)^{-1}\right] \times \left(\cos\theta_{jik} + \frac{1}{3}\right)^2$$

$$\cos\theta_{jik} = \frac{\bar{r}_{ij}^2 + \bar{r}_{ik}^2 - \bar{r}_{jk}^2}{2 \times \bar{r}_{ij} \times \bar{r}_{ik}}$$