$$\Delta G = -\frac{1}{2}\left(\frac{1}{\varepsilon_{in}} - \frac{1}{\varepsilon_{out}}\right)\sum_{i=1}^{N}\sum_{j=1}\frac{q_i q_j}{\sqrt{r_{ij}^2 + \alpha_i\alpha_j \exp\left[-\gamma \frac{r_{ij}^2}{\alpha_i\alpha_j}\right]}}$$

$$k_c' = -\frac{1}{2}\left(\frac{1}{\varepsilon_{in}} - \frac{1}{\varepsilon_{out}}\right)$$

$$G_{ij} = \frac{q_i q_j}{\sqrt{r_{ij}^2 + \alpha_i\alpha_j \exp\left[-\gamma \frac{r_{ij}^2}{\alpha_i\alpha_j}\right]}} = G_{ij}(r_{ij}, \alpha_i, \alpha_j)$$

$$\frac{1}{k_c'}\Delta G = \sum_{i=1}^{N}\sum_{j=1}^{N} G_{ij}$$

$$\frac{1}{k_c'}\nabla_e \Delta G = \underbrace{\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{m=1}^{N}\sum_{n=1}^{N}\frac{\partial G_{ij}}{\partial r_{mn}}\nabla_e r_{mn}}_{1} + \underbrace{\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_k}\nabla_e \alpha_k}_{2}$$

$$\nabla_l r_{mn} = \frac{\vec{r}_{mn}}{r_{mn}} (\delta_{lm} - \delta_{ln})$$

$$\frac{\partial G_{ij}}{\partial r_{mn}} = \frac{\partial G_{ij}}{\partial r_{mn}} \left(\delta_{mi} \cdot \delta_{nj} \right) \quad (\text{since } G_{ij} = G_{ij}(r_{ij}, \alpha_i, \alpha_j))$$

Then

$$\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{m=1}^{N}\sum_{n=1}^{N} \frac{\partial G_{ij}}{\partial r_{mn}} \cdot \nabla_l r_{mn} = \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{m=1}^{N}\sum_{n=1}^{N} \frac{\partial G_{ij}}{\partial r_{mn}} \delta_{mi}\delta_{nj} \cdot \nabla_l r_{mn} =$$

$$= \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{\partial G_{ij}}{\partial r_{ij}} \nabla_l r_{ij} = \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{\partial G_{ij}}{\partial r_{ij}} \cdot \frac{\vec{r}_{ij}}{r_{ij}} \left(\delta_{li} - \delta_{lj} \right) =$$

$$= \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{\partial G_{ij}}{\partial r_{ij}} \frac{\vec{r}_{ij}}{r_{ij}} \delta_{li} - \sum_{i=1}^{N}\sum_{j=1}^{N} \frac{\partial G_{ij}}{\partial r_{ij}} \frac{\vec{r}_{ij}}{r_{ij}} \delta_{lj} = \sum_{j=1}^{N} \frac{\partial G_{lj}}{\partial r_{lj}} \frac{\vec{r}_{lj}}{r_{lj}} - \sum_{i=1}^{N} \frac{\partial G_{il}}{\partial r_{il}} \frac{\vec{r}_{il}}{r_{il}} =$$

$$= \sum_{i=1}^{N} \frac{\partial G_{li}}{\partial r_{li}} \frac{\vec{r}_{li}}{r_{li}} - \sum_{i=1}^{N} \frac{\partial G_{il}}{\partial r_{il}} \frac{\vec{r}_{il}}{r_{il}} = \underbrace{\sum_{i=1}^{N} \frac{\partial G_{il}}{\partial r_{il}} \cdot \frac{-\vec{r}_{il}}{r_{il}} - \sum_{i=1}^{N} \frac{\partial G_{il}}{\partial r_{il}} \frac{\vec{r}_{il}}{r_{il}}}_{\text{since } G_{ij} = G_{ji},\ r_{ij} = r_{ji},\ \vec{r}_{ij} = -\vec{r}_{ji}} =$$

$$= -2 \sum_{i=1}^{N} \frac{\partial G_{il}}{\partial r_{il}} \cdot \frac{\vec{r}_{il}}{r_{il}}$$

$$\frac{\partial G_{il}}{\partial r_{il}} = q_i q_l \left(-\frac{1}{2}\right) \frac{1}{\left(r_{il}^2 + \alpha_i \alpha_l \exp\left[-\gamma \frac{r_{il}^2}{\alpha_i \alpha_l}\right]\right)^{3/2}} \left(2 r_{il} + \alpha_i \alpha_l \exp\left[-\gamma \frac{r_{il}^2}{\alpha_i \alpha_l}\right] \cdot \left(-\gamma \frac{2 r_{il}}{\alpha_i \alpha_l}\right)\right)$$

$$= q_i q_l \left(-\frac{1}{2}\right) \frac{1}{\left(r_{il}^2 + \alpha_i \alpha_l \exp\left[-\gamma \frac{r_{il}^2}{\alpha_i \alpha_l}\right]\right)^{3/2}} \cdot 2 r_{il} \left(1 - \gamma \cdot \exp\left[-\gamma \frac{r_{il}^2}{\alpha_i \alpha_l}\right]\right)$$

$$-2 \sum_{i=1}^{N} \frac{\partial G_{il}}{\partial r_{il}} \frac{\vec{r}_{il}}{r_{il}} = -2 \sum_{i=1}^{N} \frac{q_i q_l}{\left(r_{il}^2 + \alpha_i \alpha_l \exp\left[-\gamma \frac{r_{il}^2}{\alpha_i \alpha_l}\right]\right)^{3/2}} \cdot \left(-\frac{1}{2}\right) \cdot 2 r_{il} \left(1 - \gamma \exp\left[-\gamma \frac{r_{il}^2}{\alpha_i \alpha_l}\right]\right) \frac{\vec{r}_{il}}{r_{il}}$$

$$= 2 q_l \sum_{i=1}^{N} \frac{q_i \cdot \left(1 - \gamma \exp\left[-\gamma \frac{r_{il}^2}{\alpha_i \alpha_l}\right]\right)}{\left(r_{il}^2 + \alpha_i \alpha_l \exp\left[-\gamma \frac{r_{il}^2}{\alpha_i \alpha_l}\right]\right)^{3/2}} \cdot \vec{r}_{il}$$

$$\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_k}\nabla_\ell \alpha_k$$

$$\frac{\partial G_{ij}}{\partial \alpha_k} = \frac{\partial G_{ij}}{\partial \alpha_k}\cdot(\delta_{ik}+\delta_{jk}) \qquad (\text{since } G_{ij}=G_{ij}(r_{ij},\alpha_i,\alpha_j))$$

$$\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_k}\nabla_\ell \alpha_k = \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_k}(\delta_{ik}+\delta_{jk})\nabla_\ell \alpha_k =$$

$$= \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\frac{\partial G_{ij}}{\partial r_k}\delta_{ik}\nabla_\ell \alpha_k + \sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_k}\delta_{jk}\nabla_\ell \alpha_k =$$

$$= \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\nabla_\ell \alpha_i + \sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_j}\nabla_\ell \alpha_j = 2\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\nabla_\ell \alpha_i$$

$$(\text{since } G_{ij}=G_{ji})$$

$$\frac{\partial G_{ij}}{\partial \alpha_i} = \left(-\frac{1}{2}\right)\frac{q_i q_j}{\left(r_{ij}^2+\alpha_i\alpha_j\exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]\right)^{3/2}}\cdot\left(\alpha_j\exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]+\alpha_i\alpha_j\cdot\exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]\cdot\right.$$

$$\left.\cdot\left(-\gamma\frac{r_{ij}^2}{\alpha_j}\right)\cdot\left(-\frac{1}{\alpha_i^2}\right)\right) = \left(-\frac{1}{2}\right)\frac{q_i q_j}{\left(r_{ij}^2+\alpha_i\alpha_j\exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]\right)^{3/2}}\cdot\alpha_j\cdot\exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]\cdot$$

$$\cdot\left(1+\alpha_i\cdot\gamma\frac{r_{ij}^2}{\alpha_i^2\alpha_j}\right) =$$

$$= \left(-\frac{1}{2}\right)\frac{q_i q_j\cdot\alpha_j\exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]}{\left(r_{ij}^2+\alpha_i\alpha_j\exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]\right)^{3/2}}\cdot\left(1+\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right)$$

Pair-based approach

$\alpha_i = f(S_i)$, where $S_i = \sum_{k=1}^{N} \alpha_{ik}$ and $\alpha_{ik} = \alpha_{ik}(r_{ik})$

In general, $\alpha_{ij} \neq \alpha_{ji}$

Then $\nabla_\ell \alpha_i = \frac{\partial f(S_i)}{\partial S_i} \nabla_\ell S_i$

$$\nabla_\ell S_i = \nabla_\ell \sum_{k=1}^{N} \alpha_{ik} = \sum_{k=1}^{N} \nabla_\ell \alpha_{ik}$$

$$\nabla_\ell \alpha_{ik} = \frac{\partial \alpha_{ik}}{\partial r_{ik}} \delta_{i\ell} \frac{\vec{r}_{ik}}{r_{ik}} - \frac{\partial \alpha_{ik}}{\partial r_{ik}} \cdot \delta_{k\ell} \frac{\vec{r}_{ik}}{r_{ik}}$$

$$\nabla_\ell S_i = \sum_{k=1}^{N} \frac{\partial \alpha_{ik}}{\partial r_{ik}} \delta_{i\ell} \frac{\vec{r}_{ik}}{r_{ik}} - \sum_{k=1}^{N} \frac{\partial \alpha_{ik}}{\partial r_{ik}} \delta_{k\ell} \frac{\vec{r}_{ik}}{r_{ik}} =$$

$$= \sum_{k=1}^{N} \frac{\partial \alpha_{ik}}{\partial r_{ik}} \delta_{i\ell} \frac{\vec{r}_{ik}}{r_{ik}} - \frac{\partial \alpha_{i\ell}}{\partial r_{i\ell}} \cdot \frac{\vec{r}_{i\ell}}{r_{i\ell}}$$

$$\nabla_\ell \alpha_i = \frac{\partial f(S_i)}{\partial S_i} \cdot \left(\sum_{k=1}^{N} \frac{\partial \alpha_{ik}}{\partial r_{ik}} \delta_{i\ell} \frac{\vec{r}_{ik}}{r_{ik}} - \frac{\partial \alpha_{i\ell}}{\partial r_{i\ell}} \frac{\vec{r}_{i\ell}}{r_{i\ell}} \right)$$

$$2\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\nabla_l \alpha_i = 2\cdot\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\frac{\partial f(S_i)}{\partial S_i}\cdot\left(\sum_{k=1}^{N}\frac{\partial \alpha_{ik}}{\partial r_{ik}}\delta_{il}\frac{\vec{r}_{ik}}{r_{ik}} - \frac{\partial \alpha_{il}}{\partial r_{il}}\frac{\vec{r}_{il}}{r_{il}}\right) =$$

$$= 2\sum_{i=1}^{N}\sum_{j=1}^{N}\sum_{k=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\frac{\partial f(S_i)}{\partial S_i}\cdot\frac{\partial \alpha_{ik}}{\partial r_{ik}}\delta_{il}\frac{\vec{r}_{ik}}{r_{ik}} -$$

$$- 2\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\frac{\partial f(S_i)}{\partial S_i}\cdot\frac{\partial \alpha_{il}}{\partial r_{il}}\frac{\vec{r}_{il}}{r_{il}} =$$

$$= 2\sum_{j=1}^{N}\sum_{k=1}^{N}\frac{\partial G_{lj}}{\partial \alpha_l}\frac{\partial f(S_l)}{\partial S_l}\cdot\frac{\partial \alpha_{lk}}{\partial r_{lk}}\frac{\vec{r}_{lk}}{r_{lk}} -$$

$$- 2\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\frac{\partial f(S_i)}{\partial S_i}\frac{\partial \alpha_{il}}{\partial r_{il}}\frac{\vec{r}_{il}}{r_{il}} =$$

$$= 2\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{lj}}{\partial \alpha_l}\frac{\partial f(S_l)}{\partial S_l}\frac{\partial \alpha_{li}}{\partial r_{li}}\frac{\vec{r}_{li}}{r_{li}} - 2\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\frac{\partial f(S_i)}{\partial S_i}\frac{\partial \alpha_{il}}{\partial r_{il}}\frac{\vec{r}_{il}}{r_{il}} =$$

$$= -2\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{lj}}{\partial \alpha_l}\frac{\partial f(S_l)}{\partial S_l}\frac{\partial \alpha_{li}}{\partial r_{li}}\cdot\frac{\vec{r}_{il}}{r_{il}} - 2\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\frac{\partial f(S_i)}{\partial S_i}\frac{\partial \alpha_{il}}{\partial r_{il}}\frac{\vec{r}_{il}}{r_{il}} =$$

$$= -2\sum_{i=1}^{N}\left(\frac{\partial f(S_l)}{\partial S_l}\frac{\partial \alpha_{li}}{\partial r_{li}}\cdot\frac{\vec{r}_{il}}{r_{il}}\sum_{j=1}^{N}\frac{\partial G_{lj}}{\partial \alpha_l} + \frac{\partial f(S_i)}{\partial S_i}\frac{\partial \alpha_{il}}{\partial r_{il}}\frac{\vec{r}_{il}}{r_{il}}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\right) =$$

$$= -2\sum_{i=1}^{N}\left(\frac{\partial f(S_l)}{\partial S_l}\frac{\partial \alpha_{li}}{\partial r_{li}}\sum_{j=1}^{N}\frac{\partial G_{lj}}{\partial \alpha_l} + \frac{\partial f(S_i)}{\partial S_i}\frac{\partial \alpha_{il}}{\partial r_{il}}\cdot\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\right)\frac{\vec{r}_{il}}{r_{il}}$$

$$2\sum_{i=1}^{N}\sum_{j=1}^{N}\frac{\partial G_{ij}}{\partial \alpha_i}\nabla_l \alpha_i = -2\sum_{i=1}^{N}\left(\frac{\partial f(S_l)}{\partial S_l}\frac{\partial \alpha_{li}}{\partial r_{li}}\cdot\sum_{j=1}^{N}\left(-\frac{1}{2}\right)\frac{q_l q_j \alpha_j \exp\left[-\gamma\frac{r_{lj}^2}{\alpha_l\alpha_j}\right]}{\left(r_{lj}^2+\alpha_l\alpha_j\exp\left[-\gamma\frac{r_{lj}^2}{\alpha_l\alpha_j}\right]\right)^{3/2}}\left(1+\gamma\frac{r_{lj}^2}{\alpha_l\alpha_j}\right)+\right.$$

$$\left.+\frac{\partial f(S_i)}{\partial S_i}\frac{\partial \alpha_{il}}{\partial r_{il}}\cdot\sum_{j=1}^{N}\left(-\frac{1}{2}\right)\frac{q_i q_j \alpha_j \exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]}{\left(r_{ij}^2+\alpha_i\alpha_j\exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]\right)^{3/2}}\cdot\left(1+\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right)\right)\frac{\vec{r}_{il}}{r_{il}} =$$

$$= \sum_{i=1}^{N}\left(\frac{\partial f(S_l)}{\partial S_l}\frac{\partial \alpha_{li}}{\partial r_{li}}\left\{q_l\sum_{j=1}^{N}\frac{q_j\alpha_j\exp\left[-\gamma\frac{r_{lj}^2}{\alpha_l\alpha_j}\right]}{\left(r_{lj}^2+\alpha_l\alpha_j\exp\left[-\gamma\frac{r_{lj}^2}{\alpha_l\alpha_j}\right]\right)^{3/2}}\left(1+\gamma\frac{r_{lj}^2}{\alpha_l\alpha_j}\right)\right\}+\right.$$

$$\left.+\frac{\partial f(S_i)}{\partial S_i}\frac{\partial \alpha_{il}}{\partial r_{il}}\left\{q_i\sum_{j=1}^{N}\frac{q_j\alpha_j\exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]}{\left(r_{ij}^2+\alpha_i\alpha_j\exp\left[-\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right]\right)^{3/2}}\left(1+\gamma\frac{r_{ij}^2}{\alpha_i\alpha_j}\right)\right\}\right)\frac{\vec{r}_{il}}{r_{il}}$$

$$\frac{1}{k_i}\nabla_e G = 2 q_e \sum_{i=1}^{N} \frac{q_i\left(1-\gamma \exp\left[-\gamma \frac{r_{ie}^2}{\alpha_i \alpha_e}\right]\right)}{\left(r_{ie}^2+\alpha_i \alpha_e \exp\left[-\gamma \frac{r_{ie}^2}{\alpha_i \alpha_e}\right]\right)^{3/2}} \cdot \vec{r}_{ie} +$$

$$+ \sum_{i=1}^{N} \left(\frac{\partial f(S_e)}{\partial S_e} \frac{\partial \alpha_{ei}}{\partial r_{ei}} \left\{ q_e \sum_{j=1}^{N} \frac{q_j \alpha_j \exp\left[-\gamma \frac{r_{ej}^2}{\alpha_e \alpha_j}\right]}{\left(r_{ej}^2+\alpha_e \alpha_j \exp\left[-\gamma \frac{r_{ej}^2}{\alpha_e \alpha_j}\right]\right)^{3/2}} \cdot \left(1+\gamma \frac{r_{ej}^2}{\alpha_e \alpha_j}\right) \right\} + \right.$$

$$\left. + \frac{\partial f(S_i)}{\partial S_i} \frac{\partial \alpha_{ie}}{\partial r_{ie}} \cdot \left\{ q_i \sum_{j=1}^{N} \frac{q_j \alpha_j \exp\left[-\gamma \frac{r_{ij}^2}{\alpha_i \alpha_j}\right]}{\left(r_{ij}^2+\alpha_i \alpha_j \exp\left[-\gamma \frac{r_{ij}^2}{\alpha_i \alpha_j}\right]\right)^{3/2}} \left(1+\gamma \frac{r_{ij}^2}{\alpha_i \alpha_j}\right) \right\} \right) \cdot \frac{\vec{r}_{ie}}{r_{ie}}$$

$\frac{\partial f(s_i)}{\partial s_i}$ and $\frac{\partial \alpha_{ij}}{\partial r_{ij}}$

1. Still model.

$$\alpha_i = -\frac{k_c}{2 G_{pol,i}}$$

$$\Delta G_{pol,i} = \left(\frac{1}{\varepsilon_{in}} - \frac{1}{\varepsilon_{out}}\right)\left[\frac{1}{\lambda}\left(-\frac{k_c}{2}\right)\cdot\frac{1}{R_{vdw,i}} + P_1\left(\frac{k_c}{2R_{vdw,i}^2}\right) + \right.$$

$$\left. + \sum_j^{bond} \frac{P_2 V_j}{r_{ij}^4} + \sum_j^{angle} \frac{P_3 V_j}{r_{ij}^4} + \sum_j^{nb} \frac{P_4 V_j}{r_{ij}^4} CCF \right]$$

where
$$CCF = \begin{cases} 1.0 & \text{if } \left(\frac{r_{ij}}{R_{vdw,i}+R_{vdw,j}}\right)^2 > \frac{1}{P_5} \\ \left\{\frac{1}{2}\left[1-\cos\left(\left(\frac{r_{ij}}{R_{vdw,i}+R_{vdw,j}}\right)^2 P_5 \pi\right)\right]\right\}^2 & \text{otherwise} \end{cases}$$

$$\alpha_i = -\frac{k_c}{2\left(\frac{1}{\varepsilon_{in}} - \frac{1}{\varepsilon_{out}}\right)\left(\frac{1}{\lambda}\left(-\frac{k_c}{2}\right)\frac{1}{R_{vdw,i}} + P_1\left(\frac{k_c}{2R_{vdw,i}^2}\right) + \sum_{j=1}^{N} \frac{P[CCF]\cdot V_j}{r_{ij}^4}\right)}$$

Here, $P \equiv P_2, P_3$ or P_4 depending on connectivity.
$[CCF] = 1$ or CCF

$$\alpha_i = \frac{1}{-\frac{2}{k_c}\left(\frac{1}{\varepsilon_{in}} - \frac{1}{\varepsilon_{out}}\right)\left(\frac{1}{\lambda}\left(-\frac{k_c}{2}\right)\cdot\frac{1}{R_{vdw,i}} + P_1\frac{k_c}{2R_{vdw,i}^2}\right) - \frac{1}{2}\sum_{j=1}^{N} \frac{4}{k_c}\left(\frac{1}{\varepsilon_{in}} - \frac{1}{\varepsilon_{out}}\right)\cdot\frac{P\cdot[CCF]V_j}{r_{ij}^4}} =$$

$$= \frac{1}{\frac{1}{\rho_{0i}} - \frac{1}{2}\sum_{j=1}^{N} H_{ij}}$$

where
$$\rho_{0i} = \frac{1}{\left(\frac{1}{\varepsilon_{in}} - \frac{1}{\varepsilon_{out}}\right)\left(\frac{1}{\lambda R_{vdw,i}} - \frac{P_1}{R_{vdw,i}^2}\right)}$$

$$H_{ij} = \frac{4}{k_c}\left(\frac{1}{\varepsilon_{in}} - \frac{1}{\varepsilon_{out}}\right)\frac{P\,[CCF]\,V_j}{r_{ij}^4}$$

→ HCT model

$$\alpha_i^{-1} = \rho_i^{-1} - \frac{1}{2}\sum_j \left[\frac{1}{L_{ij}} - \frac{1}{U_{ij}} + \frac{r_{ij}}{4}\left(\frac{1}{U_{ij}^2} - \frac{1}{L_{ij}^2}\right) + \frac{1}{r_{ij}} \ln \frac{L_{ij}}{U_{ij}} + \frac{S_{ji}^2 \rho_j^2}{4 r_{ij}}\left(\frac{1}{L_{ij}^2} - \frac{1}{U_{ij}^2}\right)\right]$$

$$L_{ij} = \begin{cases} 1 & \text{if } r_{ij} + S_{ji}\rho_j \le \rho_i \\ \rho_i & \text{if } r_{ij} - S_{ji}\rho_j \le \rho_i < r_{ij} + S_{ji}\rho_j \\ r_{ij} - S_{ji} & \text{if } \rho_i \le r_{ij} - S_{ji}\rho_j \end{cases}$$

$$\boxed{\frac{\partial f}{\partial S} = \frac{\partial}{\partial S}\left(\frac{1}{\frac{1}{\rho_i} - \frac{1}{2}S}\right) = -\frac{1}{\left(\frac{1}{\rho_i} - \frac{1}{2}S\right)^2}\left(-\frac{1}{2}\right) S = \frac{1}{2}\alpha^2 S}$$

$$U_{ij} = \begin{cases} 1 & \text{if } r_{ij} + \rho_{ji} \le \rho_i \\ r_{ij} + S_{ji}\rho_j & \text{if } \rho_i < r_{ij} + S_{ji}\rho_j \end{cases}$$

$$\alpha_i = \frac{1}{\frac{1}{\rho_i} - \frac{1}{2}\sum_{j \ne i}^{N} \alpha_{ij}} = \frac{1}{\frac{1}{\rho_i} - \frac{1}{2}S_i} = f(S_i)$$

$$\frac{\partial f(S_i)}{\partial S_i} = \frac{-1}{\left(\frac{1}{\rho_i} - \frac{1}{2}S_i\right)^2} \cdot \left(-\frac{1}{2}\right) = \frac{1}{2\left(\frac{1}{\rho_i} - \frac{1}{2}S_i\right)^2} = \frac{\alpha_i^2}{2}$$

$$\alpha_{ij} = \frac{1}{L_{ij}} - \frac{1}{U_{ij}} + \frac{r_{ij}}{4}\left(\frac{1}{U_{ij}^2} - \frac{1}{L_{ij}^2}\right) + \frac{1}{r_{ij}} \ln \frac{L_{ij}}{U_{ij}} + \frac{S_{ji}^2 \rho_j^2}{4 r_{ij}}\left(\frac{1}{L_{ij}^2} - \frac{1}{U_{ij}^2}\right)$$

$$\frac{\partial \alpha_{ij}}{\partial r_{ij}} = -\frac{1}{L_{ij}^2}\frac{\partial L_{ij}}{\partial r_{ij}} + \frac{1}{U_{ij}^2}\frac{\partial U_{ij}}{\partial r_{ij}} + \frac{1}{4}\left(\frac{1}{U_{ij}^2} - \frac{1}{L_{ij}^2}\right) + \frac{r_{ij}}{4}\left(-\frac{2}{U_{ij}^3}\frac{\partial U_{ij}}{\partial r_{ij}} + \frac{2}{L_{ij}^3}\frac{\partial L_{ij}}{\partial r_{ij}}\right) +$$

$$+ \frac{-1}{r_{ij}^2} \ln \frac{L_{ij}}{U_{ij}} + \frac{1}{r_{ij}} \cdot \frac{U_{ij}}{L_{ij}}\left(\frac{1}{U_{ij}}\frac{\partial L_{ij}}{\partial r_{ij}} - \frac{L_{ij}}{U_{ij}^2}\frac{\partial U_{ij}}{\partial r_{ij}}\right) +$$

$$+ \frac{-S_{ji}^2 \rho_j^2}{4 r_{ij}^2}\left(\frac{1}{L_{ij}^2} - \frac{1}{U_{ij}^2}\right) + \frac{S_{ji}^2 \rho_j^2}{4 r_{ij}} \cdot \left(-\frac{2}{L_{ij}^3}\frac{\partial L_{ij}}{\partial r_{ij}} + \frac{2}{U_{ij}^3}\frac{\partial U_{ij}}{\partial r_{ij}}\right)$$

$$a_{ij} = \left(\frac{1}{L_{ij}} - \frac{1}{U_{ij}}\right) + \left(\frac{1}{U_{ij}^2} - \frac{1}{L_{ij}^2}\right)\left(\frac{r_{ij}}{4} - \frac{S_{ji}^2 \rho_j^2}{4 r_{ij}}\right) + \frac{1}{2 r_{ij}} \ln \frac{L_{ij}}{U_{ij}} =$$

$$= \left(\frac{1}{L_{ij}} - \frac{1}{U_{ij}}\right) + \frac{1}{4}\left(\frac{1}{U_{ij}^2} - \frac{1}{L_{ij}^2}\right)\left(r_{ij} - \frac{S_{ji}^2 \rho_j^2}{4 r_{ij}}\right) + \frac{1}{2 r_{ij}} \ln \frac{L_{ij}}{U_{ij}}$$

$$\frac{\partial a_{ij}}{\partial r_{ij}} = -\frac{1}{L_{ij}^2}\frac{\partial L_{ij}}{\partial r_{ij}} + \frac{1}{U_{ij}^2}\frac{\partial U_{ij}}{\partial r_{ij}} + \frac{1}{4}\left[\left(-\frac{2}{U_{ij}^3}\frac{\partial U_{ij}}{\partial r_{ij}} + \frac{2}{L_{ij}^3}\frac{\partial L_{ij}}{\partial r_{ij}}\right)\left(r_{ij} - \frac{S_{ji}^2 \rho_j^2}{r_{ij}}\right) +\right.$$

$$\left. + \left(\frac{1}{U_{ij}^2} - \frac{1}{L_{ij}^2}\right)\left(1 + \frac{S_{ji}^2 \rho_j^2}{r_{ij}^2}\right)\right] - \frac{1}{2 r_{ij}^2} \ln \frac{L_{ij}}{U_{ij}} +$$

$$+ \frac{1}{r_{ij}} \cdot \frac{U_{ij}}{L_{ij}} \cdot \left(\frac{1}{U_{ij}}\frac{\partial L_{ij}}{\partial r_{ij}} - \frac{L_{ij}}{U_{ij}^2} \cdot \frac{\partial U_{ij}}{\partial r_{ij}}\right) =$$

$$= -\frac{1}{L_{ij}^2}\frac{\partial L_{ij}}{\partial r_{ij}} + \frac{1}{U_{ij}^2}\frac{\partial U_{ij}}{\partial r_{ij}} + \frac{1}{2}\left(-\frac{1}{U_{ij}^3}\frac{\partial U_{ij}}{\partial r_{ij}} + \frac{1}{L_{ij}^3}\frac{\partial L_{ij}}{\partial r_{ij}}\right)\left(r_{ij} - \frac{S_{ji}^2 \rho_j^2}{r_{ij}}\right) +$$

$$+ \frac{1}{4}\left(\frac{1}{U_{ij}^2} - \frac{1}{L_{ij}^2}\right)\left(1 + \frac{S_{ji}^2 \rho_j^2}{r_{ij}^2}\right) - \frac{1}{2 r_{ij}^2} \ln \frac{L_{ij}}{U_{ij}} + \frac{1}{r_{ij}}\left(\frac{1}{L_{ij}}\frac{\partial L_{ij}}{\partial r_{ij}} - \frac{1}{U_{ij}}\frac{\partial U_{ij}}{\partial r_{ij}}\right)$$

$$Ul_0 = \frac{1}{U_{ij}^2} - \frac{1}{L_{ij}^2}$$

$$Ul_1 = \frac{1}{r_{ij}}\left(-\frac{1}{2 r_{ij}} \ln \frac{L_{ij}}{U_{ij}} + \left(\frac{1}{L_{ij}}\frac{\partial L_{ij}}{\partial r_{ij}} - \frac{1}{U_{ij}}\frac{\partial U_{ij}}{\partial r_{ij}}\right)\right)$$

$$Ul_2 = -\frac{1}{L_{ij}^2}\frac{\partial L_{ij}}{\partial r_{ij}} + \frac{1}{U_{ij}^2}\frac{\partial U_{ij}}{\partial r_{ij}} \qquad Ul_3 = -\frac{1}{U_{ij}^3}\frac{\partial U_{ij}}{\partial r_{ij}} + \frac{1}{L_{ij}^3}\frac{\partial L_{ij}}{\partial r_{ij}}$$

$$\frac{\partial a_{ij}}{\partial r_{ij}} = \frac{1}{4} Ul_0 \cdot \left(1 + \frac{S_{ji}^2 \rho_j^2}{r_{ij}^2}\right) + Ul_1 + Ul_2 + \frac{1}{2} Ul_3 \cdot \left(r_{ij} - \frac{S_{ji}^2 \rho_j^2}{r_{ij}}\right)$$

GOBC model

$$\alpha_i^{-1} = \tilde{\rho}_i^{-1} - \rho_i^{-1} \tanh(\alpha \Psi_i - \beta \Psi_i^2 + \gamma \Psi_i^3)$$

- $\Psi_i = I \cdot \tilde{\rho}_i = \frac{1}{2} S \tilde{\rho}_i$

$\tilde{\rho}_i = \rho_i - 0.09 Å$

$$\frac{\partial f}{\partial S} = \frac{\partial}{\partial S}\left(\frac{1}{\frac{1}{\tilde{\rho}_i} - \frac{1}{\rho_i} \cdot \tanh(\alpha \frac{1}{2} S \tilde{\rho}_i - \beta (\frac{1}{2} S \tilde{\rho}_i)^2 + \gamma \cdot (\frac{1}{2} S \tilde{\rho}_i)^3)} \right) =$$

$$= -\frac{1}{(\quad)^2} \cdot \left(-\frac{1}{\rho_i}\right) \cdot \left(1 - \tanh^2(\alpha - \beta \cdot \gamma)\right) \cdot$$

$$\cancel{\cdot \frac{1}{2} \alpha \tilde{\rho}_i - 2 \cdot \frac{1}{4} \tilde{\rho}_i^2 S^2 + \frac{3}{8} \gamma (S^3 \tilde{\rho}_i^3)} =$$

$$= \cancel{\alpha_i^2 \frac{1}{\rho_i} (1 - \tanh^2)} \cdot$$

$$\cdot \left(\alpha \cdot \frac{1}{2} \tilde{\rho}_i - \beta \frac{2}{4} S \tilde{\rho}_i^2 + \gamma \frac{3}{8} S^2 \tilde{\rho}_i^3 \right) =$$

$$= \frac{\alpha_i^2}{\rho_i} \cdot (1 - \tanh) \cdot \frac{\tilde{\rho}_i}{2} \left(\alpha - \beta S \tilde{\rho}_i + \gamma \frac{3}{4} (S \tilde{\rho}_i)^2 \right) \cdot$$

$$= \frac{\alpha_i^2}{\rho_i} (1 - \tanh^2) \tilde{\rho}_i \left(\frac{1}{2} \alpha - \beta \left(\frac{1}{2} S \tilde{\rho}_i\right) + \gamma \frac{3}{2} \left(\frac{1}{2} S \tilde{\rho}_i\right)^2 \right)$$