Problem I: SiO_2 Potential

In class we have determined the force $\vec{F}_i$ on a particle i for a system with Lennard-Jones interactions. These forces are the core of the molecular dynamics simulations I ran and analyzed in the past in my research. Another system which I study lately is SiO_2, which is the main component of window glass (a very cool system!). During the last twenty years the following BKS Potential [Phys. Rev. Lett. **64**, 1955 (1990)] has been shown to be a good model for real SiO_2:

$$U_{ij}(r_{ij}) = \frac{q_i q_j \mathrm{e}^2}{r_{ij}} + A_{ij} \exp\left(-B_{ij} r_{ij}\right) - \frac{C_{ij}}{r_{ij}^6}$$

where $r_{ij} = |\vec{r}_i - \vec{r}_j|$ and q_i, A_{ij}, B_{ij}, and C_{ij} are constants. Similar to the calculation in class, determine the force $\mathbf{F}_i$ on particle i due to all other particles $j = 1, \ldots, N$. [1]

[1] To tell the whole truth, since the Coulomb force is long ranged, the actual calculation of this term is in practice more complicated.