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Zero Internal Concentration Polarization FO Membrane: Functionalized Graphene

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COMPASS force-field

The empirical function forms of the COMPASS force-field model are described as follows:

$$
\begin{aligned}
E_{total} = & \sum_{b}[k_2(b-b_0)^2 + k_3(b-b_0)^3 + k_4(b-b_0)^4] \\
& + \sum_{\theta}[k_2(\theta-\theta_0)^2 + k_3(\theta-\theta_0)^3 + k_4(\theta-\theta_0)^4] \\
& + \sum_{\phi}[k_1(1-\cos\phi) + k_2(1-\cos 2\phi) + k_3(1-\cos 3\phi)] \\
& + \sum_{\chi} k_2(\chi-\chi_0)^2 \\
& + \sum_{b,b'} k(b-b_0)(b'-b_0') \\
& + \sum_{b,\theta} k(b-b_0)(\theta-\theta_0) \\
& + \sum_{b,\phi}(b-b_0)[k_1\cos\phi + k_2\cos 2\phi + k_3\cos 3\phi] \\
& + \sum_{b,\phi}(\theta-\theta_0)[k_1\cos\phi + k_2\cos 2\phi + k_3\cos 3\phi] \\
& + \sum_{\theta,\theta'} k(\theta-\theta_0)(\theta'-\theta_0') \\
& + \sum_{\theta,\theta',\phi} k(\theta'-\theta_0')(\theta-\theta_0)(\phi-\phi_0) \\
& + \sum_{i,j}\frac{q_i q_j}{r_{ij}} \\
& + \sum_{i,j}\varepsilon_{ij}\left[2\left(\frac{r_{ij}^0}{r_{ij}}\right)^9 - 3\left(\frac{r_{ij}^0}{r_{ij}}\right)^6\right]
\end{aligned}
\tag{1}
$$

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where, E_b, E_θ, E_ϕ, and E_χ are the valence terms for bond, angle, torsion, and out-of-plane angle coordinates, respectively, and $E_{bb'}$, $E_{b\theta}$, $E_{b\phi}$, $E_{\theta\theta'}$ and $E_{\theta\theta'\phi}$ are the cross-coupling terms between internal coordinates. q_i and q_j denote the atom charges. The nonbonded terms are described by a Coulombic term for the electrostatic interactions and by a Lennard-Jones 9-6 (L-J) potential for the vdW interaction. These L-J parameters including ε and r^0 for like atom pairs are adjustable parameters. For unlike atom pairs, these off-diagonal parameters are calculated by a sixth-order combination law which is given by,

$$r_{ij}^0 = \left(\frac{\left(r_{ii}^0\right)^6 + \left(r_{jj}^0\right)^6}{2} \right)^{\frac{1}{6}}, \qquad \varepsilon_{ij} = 2\sqrt{\varepsilon_{ii}\varepsilon_{jj}} \left[\frac{\left(r_{ii}^0 r_{jj}^0\right)^3}{\left(r_{ii}^0\right)^6 + \left(r_{jj}^0\right)^6} \right] \tag{2}$$

where, r_{ij} is the inter-atom distance. For further information about the COMPASS force-field, please see ref [1,2].

References

[1] Compass by Accelrys used Materials Studio and Cerius2 software package. http://accelrys.com/.

[2] Sun, H. *J. Phys. Chem. B* **1998**, *102*, 7338−7364.