1.The convergence plot of system

In this work, the convergence was assessed in the geometry optimization, and the Material Studio 7.0 will give the convergence plot of system. From the following picture we can see that the system tends to converge and get stable gradually with the increase of optimization step, thus the model we established can be used for molecular dynamics (MD) simulation.

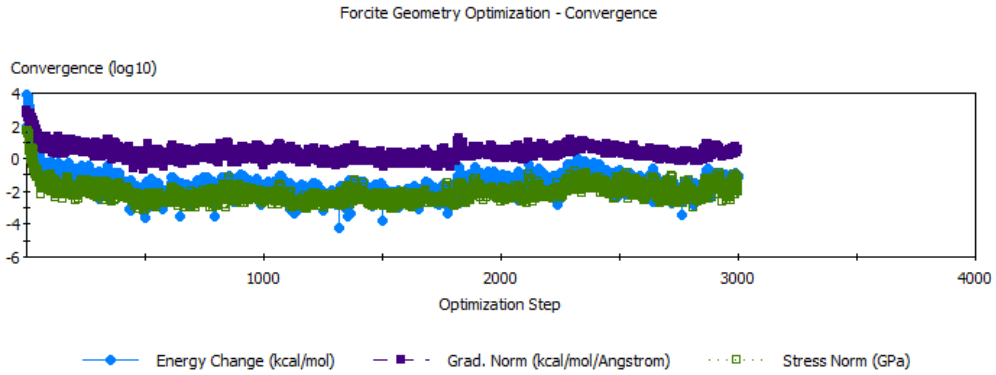

Figure 1. The convergence plot of system.

2. Calculation method and standard error of diffusion coefficient

Firstly, according to MD simulation result the MSD curve is outputted from the last 100 ps of NVT simulation (Figure 2, Take Na-MT1$_{6\text{-}0}$ as an example). Secondly, the regression equation is obtained by linear fitting the MSD curve using Origin 9.0. The one-sixth of the slope of regression equation is diffusion coefficient, and standard error can also be seen in Figure 3**.**

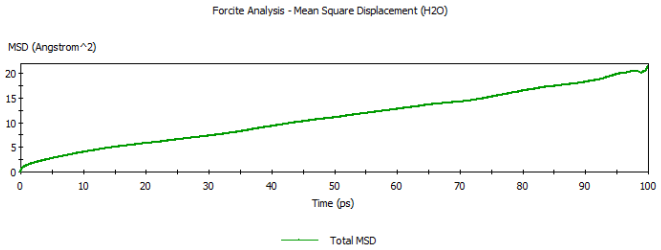

Figure 2. MSD curve of H_2O in Na-MT1$_{6\text{-}0}$.

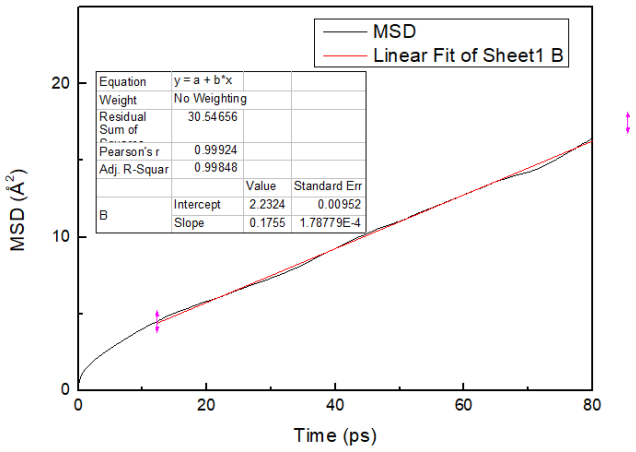

Figure 3. Regression equation of the MSD curve in Origin 9.0.