4P092

Potential of mean force between two likely charged particles in electrolyte solution

Department of Applied Chemistry , Nagoya University **
○Nurul Najwa**, Endo Yuuta**, Kojima Hidekazu**, Susumu Okazaki**,
Shinoda Wataru**, Fujimoto Kazushi**

[Introduction]

A molecular dynamics study on interaction between Polio virus and CD155 receptor using MD calculation showed that an attractive force is likely to work between them regardless of like charges .Objective of this study is to clarify an origin of the attractive force between virus and receptor base on smaller and simpler model system.

[Calculation]

Calculations have been done for a model system consisting of two uniformly charged spheres . A large sphere (sphere 1) with radius of R_1=24.4A and surface charge density , σ=-1.07 ×10^{17} e/m^2 models a virus while a small sphere (sphere 2) with radius of R_2=5.0A models receptor . Since the charges on the virus model is considered to play an important role in producing attractive force , the value of the charge is set to mimic the surface charge density of the real virus giving us an uniformly charged sphere of total charge of -8e while for the receptor model, the total charged was set to be -2e. Both spheres are immersed in monovalent 1:1 electrolyte solution mimicking the ionic strength of the phosphate-buffered saline (PBS) at neutral pH7.4. In this calculation , the cations and anions of the PBS solution are replaced by 28 sodium ions , 28 chloride ions and additional 10 sodium ions to neutralize net excess 10 negative charges of the two spheres discussed above. The total number of atom is 20633 including water molecules.

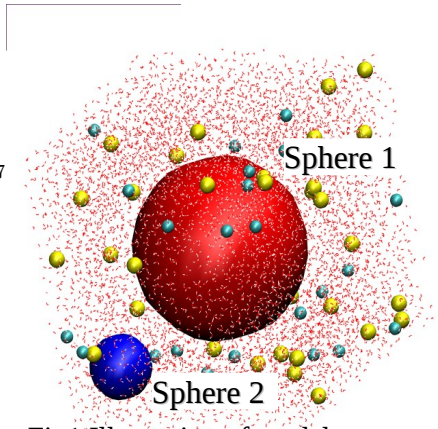

Fig1 Illustration of model system

The MD calculations were carried out in the NPT ensemble at pressure of 1atm and temperature of 310.15K . The Lennard-Jones (LJ) cut off was 12A and

long ranged interaction was calculated using Ewald summation with sufficient reciprocal space calculation for the present anisotropic system.

Wall potentials were introduced to both spheres .

$$U(r) = \sum_i \sum_j \frac{Q_i q_j}{4\pi\varepsilon_0} \cdot \frac{1}{r_{ij}} + \sum_i \sum_j \varepsilon_j \left(\frac{\sigma_j}{r_{ij} - l_j} \right)^{12}$$

where i represent the spheres 1 and 2 and j the atoms of solvent water and ions , Q_i the charge of the spheres , q_j the charge of solvent atoms.Here ,we adopted σ =1.00 [Å] and ε = 0.07 [kcal/mol]. r_{ij} is the distance between center of the spheres and the solvent atom .

The calculations have been done ,distance between two spheres being fixed and the force between them was observed . In this study , 13 distances between center of spheres , 30.4A, 31.4A, 32.4A, 33.4A, 35.4A, 36.4,A 37.4A, 38.4A, 39.4A, 40.4,A 41.4A, and 42.4A were examined.

[Result and discussion]

Our preliminary calculations shows that the mean force, <F> between two spheres was attractive in spite of the like charges and ,thus, the strong repulsive coulombic force between them. Here , the mean force is almost zero when two spheres are far apart , but becomes attractive as the distance between them decrease and passes through a minimum at distance of 33.4A.

This potential of mean force presents a free energy profile,ΔG asa function of distance between two spheres. It gives a solvent induced bond with the energy of -50 kJ/mol.Details are now being analyzed.